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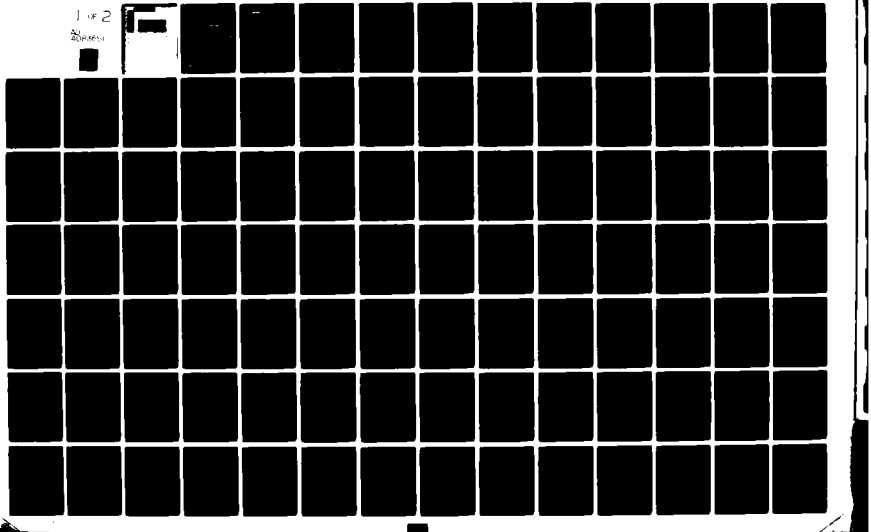

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HETEROGENEOUS COMBUSTION	CATALYTIC COMBUSTION	SUPERSONIC COMBUSTION
FLAME EXTINGUISHMENT	RAPID EXPANSION BURNING	COMBUSTION KINETICS
COMBUSTION INSTABILITY	DETONATION	ALTERNATE FUELS

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The report consists of a collection of abstracts of the numerous research progress reports given by AFOSR contractors and of invited papers from other governmental agencies and contractors. These papers presented over a five-day period composed the 1979 annual contractors meeting on Air-Breathing Combustion Dynamics and Kinetics. The principal investigators and their organizational association are also identified.

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Army Supported Research, Development Trends and Research Needs in Air Breathing Combustion

James J. Murray

U.S. Army Research Office
P. O. Box 12211
Research Triangle Park, N.C. 27709

Research in this area is undertaken in support of the following Army needs for improved and new technology: better air and ground vehicle power plants and the conservation of fuels; more efficient fixed base power plants and auxiliary power units; superior propellants needed to fire and propel projectiles and rockets; and more powerful power sources to provide the energy required for high energy weapons such as lasers. Included in this program are both theoretical and experimental studies on problems directly related to the power plants or sources required.

A superior basic understanding of the technical behavior of power plants, propellants and fuels under various conditions in which the modern Army must operate is of considerable importance to achieve needed performance in terms of agility, firepower, conservation of materials and fuels, and reduction of logistic supplies needed for effective operations. Consequently, research in energy conversion, thermodynamics, heat transfer, structures, materials, fluid mechanics, fuels, and energetic materials is most appropriate and necessary. Research is concentrated in these areas to provide the fundamental knowledge and technology for new concepts necessary to meet the Army's requirement.

The DARCOM laboratories and the Army Research Office are interested in the topics below:

Engine and Fuel Conservation: Vehicle engines and fuels must be understood if better performance, greater reliability, safety, lower maintenance, and more efficient fuel useage can be obtained for both ground vehicles and Army aircraft propulsion systems as well as other mobile and stationary power generating plants. This program requires fundamental studies in engine combustion, heat transfer, thermodynamics, materials, fluid dynamics and chemical reactions to achieve a basic understanding of the interactions of phenomena occurring in internal combustion engines versus the fuel utilized.

Propellants: The Army requires knowledge in the broad field of propellants, both for the launching and propulsion of missiles, rockets, and projectiles. Insofar as propellants are concerned, it is necessary to predict the ignition, burning, temperature and other rate effects such as pressure and volume changes, in order to obtain maximum and optimal conditions in the gun-missile systems. These needs call for basic understanding of all the interrelated phenomena from the standpoint of heat and mass transfer, thermodynamics, materials, chemical kinetics, fluid mechanics and shock and vibrations.

In view of the increasing scarcity of domestic fuel reserves, increasing vulnerability of foreign fuel resources, and rising fuel costs, the efficiency of fuel combustion processes must be decidedly improved. In addition, engine types that can satisfactorily operate on different types of fuel must be developed and explored. Particular emphasis is placed on the diesel, turbine and standard carburetor-type engines; however, new and innovative engine concepts should also be examined. These objectives require research emphasis on engine combustion, fuel flow optimization in the cylinder chamber, and an improved basic understanding of the minimally required crude oil refinement processes.

This presentation outlines and discusses the several Army activities that carry out the various vehicle R&D aspects that are identified with the topics in question, namely: the Propulsion Group of the Army Tank Automotive Research and Development Command (TARADCOM), the Army Aviation Research and Development Command (AVRADCOM), the Army Mobility Engineering Research and Development Command (MERADCOM), and the Army Research Office (ARO), (Engineering, Chemistry, and Mathematics Divisions). With respect to propellants, the Army laboratories pursuing the missile weaponry aspects are the Ballistic Research Laboratory (BRL), the Large Caliber Weapon Systems Laboratory (LCWSL), and the Army Missile Command (MICOM).

NAVY SUPPORTED RESEARCH AND NEEDS IN AIR-BREATHING COMBUSTION

J. R. Patton

Office of Naval Research
(ONR)

Abstract not received

AFRPL Supported Research and Needs Associated with Multiphase Chemically Reacting Flow Systems

D. Mann

Air Force Rocket Propulsion Lab (AFAPL)
(In house)

Abstract not received

DOE SUPPORTED RESEARCH AND NEEDS IN BASIC ENERGY SCIENCES ASSOCIATED WITH AIR-BREATHING COMBUSTION DYNAMICS AND KINETICS

O. W. Adams

Office of Basic Energy Sciences (BES)
U.S. Department of Energy
Washington, D.C. 20545

The BES/USDOE Combustion research program is composed of projects in the areas of combustion diagnostics, chemical kinetics, modeling, fluid dynamics and theory. The level of effort is about $4.5M in FY 1979 and will grow significantly in FY 1980. It covers projects in two divisions of BES, the Division of Chemical Sciences and the Division of Engineering, Mathematics and Geosciences.

A major component of the program is the large effort at the Sandia Livermore Laboratory. That effort will be described separately at this meeting. It accounts for most of the DOE-supported research and development in combustion diagnostics but it includes also a sizable basic flame research project.

The chemical kinetics projects supported by BES range from those using the molecular beam technique to those using shock tubes and includes also a kinetic data evaluation project at the NBS. Most of the individual projects are concerned with the combustion of aliphatic hydrocarbons but increasing attention is being given to the reaction involving aromatic hydrocarbons. Increased emphasis is also being given to research aimed at understanding the mechanism of soot formation.

The combustion modeling component of the program is small at the present time. The emphasis is on the mathematical aspects of modeling but we hope to expand our efforts here as an expression of the need to apply modeling as a tool to deal with complex systems.

The BES effort in fluid dynamics is small but growing. The emphasis is given primarily to fluid dynamics related to combustion modeling and accordingly includes experimental and theoretical aspects of turbulence, mixing and two phase flow. Other aspects include particle dynamics, fluidization, gas-solid reaction and catalysis.

The theoretical component of the combustion program is largely in the application of quantum chemical techniques to the study of reactions important in combustion. It is being carried out largely by investigators at the national laboratories but includes a growing number of university researchers. An interesting collaborative effort has developed involving these investigators and they have formed an ad hoc group that plans to meet three times a year to discuss their accomplishments and plans. Their ambitious plans call for a systematic study of the collision dynamics of the system of reactions involving carbon, hydrogen and oxygen.

NASA SUPPORTED RESEARCH AND NEEDS IN AIRBREATHING COMBUSTION

Donald A. Petrash

Combustion Branch
NASA Lewis Research Center
Cleveland, Ohio 44135

The combustion research and technology programs that are conducted and supported by the Combustion Branch cover a wide spectrum from the most basic studies of combustion phenomena to the evaluation of advanced combustor concepts. The overall thrust of the effort is to provide the combustion designer with the information and data required to design and develop advanced combustion systems that have high performance, reduced pollutant emissions and the capability to operate on broad specification fuels.

The overall program of combustion research and technology is conducted in-house at the Lewis Research Center, through grants to universities and through contracts with industry. At the present time the ongoing activities in combustion fundamentals are exclusively grant supported. The areas receiving the greatest attention are combustion chemistry, combustion dynamics, two-phase flow and modeling.

The fundamental research efforts have several objectives, the first of which is to gain an improved understanding of the inter-relationships of the disciplines of fluid mechanics, heat transfer and chemistry in the combustion process. The second objective is the development of analytic representations of fundamental phenomena verified by benchmark experiments thereby providing verified models of selected aspects of the overall combustion process. Lastly, to provide a data base of fundamental information and analytic design tools for the combustion system designer.

The efforts in combustion chemistry focus on the detailed rate constants and the mechanisms occurring within the combustion process. Shock tube and small scale flame tube experiments are commonly used in these studies.

Research in the area of two-phase flow is associated with fuel injection, fuel air mixing and droplet vaporization as well as the impact of these phenomena on the combustion process. Small scale flame tube experiments coupled with laser diagnostics to measure droplet size and velocity are utilized.

The combustion modeling effort will focus on the development of analytic representations of the fundamental phenomena occurring in the combustion process. Models of individual phenomena will be verified with appropriate benchmark experiments. These verified models will form the subcomponents of an integrated combustor model.

The area of combustion dynamics includes all other aspects of the combustion fundamentals program such as turbulence, combustion oscillations and combustion system transient behavior. It is in this area that the experimental development and exploitation of advanced diagnostic techniques is expected to yield information and insight previously unattainable.

NBS SUPPORTED RESEARCH RELEVANT TO AIR BREATHING COMBUSTION AND KINETICS OF AIR FORCE INTEREST

Robert S. Levine

Center for Fir Research/NBS
Washington, D. C.

Intro: NBS can be likened to an AF or NASA center that serves the Civilian sector. Research, primarily in physics and chemistry, has always been an important part of the NBS program, but there are also output oriented centers in the Bureau. These are integrated with the voluntary standards system and the various governmental agencies that have regulatory or standards setting responsibilities. As a part of the Department of Commerce, NBS is concerned also with scientific and technologically oriented problems that affect the economy and are within its competence.

Combustion research is carried out in several parts of the Bureau. These have differing missions. I will first describe the research efforts, then applied ones, and attempt to relate each to Air Force goals.

Dr. Dave Garvin and his colleagues in the Chemical Kinetics Division have long performed research in kinetics and they critically evaluate the world's kinetic data. There is a long history of close cooperation with the Air Force Office of Scientific Research in this work.

Experimental research on kinetic processes in flames is carried out in two places: by Dr. John Hastie in the Chemical Stability and Corrosion Division and Drs. Mallard and Smyth in the Center for Fire Research. Hastie probes premixed gaseous flames with and without retardants for free radicals and other species present in various zones. He has new equipment that can obtain data from flames at atmospheric pressure and that can contend with particulates in the flame. The CFR research includes exciting specific species with a tunable laser to look at the generation of possible particulate precursors. The particulate work may be of interest to the Air Force because of the environmental importance of particulates from air-breathing engines.

Incidentally, the Center for Fire Research has a significant in-house and grant program on the generation, aging, and measurement of particulates. This is of importance in fire detection and flame radiation, as well as environmentally.

Non-premixed combustion research is performed in two places: the Center for Fire Research, and the Thermal Processes Division under Drs. Ken Kreider, H. Semerjian and A. Macek. The Thermal Process Division has

a large scale model furnace equipped for both conventional and laser-related instrumentation. Teamed with a flat flame burner for debugging instruments, the purpose is to develop modern instrument techniques that can be used in industry for combustion diagnostics. The Air Force has pioneered in adapting laser-related laboratory techniques to field measurements, and we hope our work will contribute.

Two projects at the Center for Fire Research, under Dr. Kashiwagi, are of direct joint interest, and one project is jointly funded by NBS and the Air Force. The jointly funded work looks at the influence of thermal radiation from a laser or a black body source on a solid combustible material. It is found that ignition takes place in the gas phase as the gaseous decomposition products mix with air and absorb thermal energy from the source. At the same time this gaseous energy absorption partially shields the solid substrate. Dr. Kashiwagi will report in detail during this conference. His second program, which is in its early stages, is to use modern laser-related instrumentation to analyze the mixing of air and fuel gas in a jet with and without combustion. We are concerned with following the details of the process in space and time, rather than average values.

Averaged values of concentration and temperature are well known in jets where one stream enters the other reactant with appreciable momentum. In fires, whether over a burning item of furniture in a residence, of a spilled pool of jet fuel near an aircraft, the initial momentum in the buoyant unmixed flow is small, and the combustion rates, radiation from the flame, and smoke produced are quite different. Work on this subject is a part of the Center for Fire Research in-house and grant program. The results are needed for accurate mathematical modeling of the growth of fires in compartments, which is also applicable to Air Force and FAA safety concerns.

UK Supported Research, Development Trends and Research Needs in the Areas of Air-Breathing Combustion and Kinetics

G. Hooper
British Embassy
Defense Research & Development Staff

Abstract not received

RESEARCH ON RAMJET COMBUSTION AT AFAPL

R. R. Craig, R. S. Boray and F. D. Stull

Air Force Aero Propulsion Laboratory
Ramjet Engine Division
Ramjet Technology Branch
Wright-Patterson AFB, Ohio 45433

Dump combustors have become the basis for modern volume limited ramjet missile designs. Since the combustor must contain the rocket boost propellant in an integral rocket/ramjet design, use of conventional can combustors is not permitted. Flame stabilization must depend to a large extent on the recirculation zone formed by the sudden area change at the inlet duct, combustor junction. Although many such combustors have been successfully built and tested over the past several years, the specific nature of these prior designs have precluded obtaining a sound technical data base or detailed flowfield data necessary for combustor modeling efforts. The objective of the in-house research programs being conducted by the Ramjet Engine Division of the Air Force Aero Propulsion Laboratory is to provide such a data base for the development of compact ramjet combustors having wide ignition limits, high combustion efficiencies and low total pressure losses over a wide range of flight conditions, and to provide detailed data for combustion modeling studies.

An experimental investigation was conducted involving coaxial dump combustors with two different types of flameholders (annular and Y) installed at the dump station in an attempt to correlate combustor performance with previous non-reacting flowfield results. Flameholder blockage, combustor length, exit area ratio, inlet temperature, and chamber pressure were varied for both wall injection and premixed fuel conditions. Lean blowout limits, combustion efficiency, combustor total pressure drop, and wall static pressure distribution were obtained from these runs using JP-4 fuel. In addition, a limited amount of surface heating patterns and combustion oscillation data were obtained. Results from this investigation indicated the following:

1. Performance characteristics of the two types of flameholders were very different with the annular flameholder showing less sensitivity to f/a and L/D but a much greater dependency upon inlet air temperature. This suggests that a more effective flameholder could be designed by combining features of both types of flameholders.

2. Conducting premixed and wall injection tests consecutively can provide insight into the sensitivity of fuel penetration, atomization and vaporization effects on combustor performance.

3. The use of wall static pressure distribution as the sole basis for predicting overall combustor behavior is not sufficient without additional supporting data.

4. Surface heating patterns, obtained by using bare wall combustors, can be of value in developing ramburner thermal protection system and may also be useful in describing features of the combustor flowfield.

5. Adequate high frequency pressure instrumentation is essential for detecting the occurrence of combustor oscillations which can affect combustor performance and durability. Combustor screech has profound effects on combustor performance as well as producing very high local heating rates. Low frequency oscillations appear to have little influence on combustor performance but can impact inlet stability margins.

6. Detailed cold flow mixing results are useful in predicting overall combustor trends for mixing limited configurations.

Parametric combustor tests were also carried out with a variable angle swirler to determine its effect on the performance of a ramjet combustor. Swirler angles were varied from 0 to 30°, combustor length to diameter ratios from 1.5 to 3, inlet to combustor area ratios from 25 to 45% and nozzle throat to combustor area ratios from 40 to 50%. Flow into the combustor was probed in the non-burning cases to determing local flow angles as a function of swirl vane setting and also to determine when local centerline flow reversal occurred. Water tunnel flow visualization studies were made to determine flow patterns at various swirl vane settings. High speed movies were also taken of the combustion process in a transparent quartz chamber at various swirl angles. Results from this investigation showed the swirl has a dramatic effect on ramjet dump combustor performance and reduces the length of the combustion region by a factor of 2 in comparison with the non-swirl case. Future efforts are continuing in this area with new swirler designs in order to decrease total pressure losses and allow the swirl mechanism to be used in a practical ramjet dump combustor configuration.

Interfacing of the laser velocimeter counter-type processor to the Mod Comp Data Acquisition system has been completed. Software for the collection and temporary storage of individual particle velocities have been completed as well as programs for calculating first thru fourth moments and the plotting of histograms of the individual data points. Initial results clearly demonstrate the necessity for computer processing of LDV data to eliminate erroneous data points.

Single component measurements of axial and radial velocity and turbulence profiles in a cold flow dump combustor model have been completed; however, computer hardware and/or software problems have raised some doubt as to the absolute validity of the data since the integrated velocity profiles yield mass flow errors of $\pm$8%.

Future emphasis will be placed on characterizing the flowfield of a dual inlet dump combustor for ducted rocket applications, combustor instability investigations, and applying the laser velocimeter and on-line gas sampling to reactive flowfields.

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Injection, Atomization, Ignition and Combustion of Liquid Fuels in High-Speed Airstreams (AFOSR-78-3485)

J. A. Schetz and A. K. Jakubowski
Virginia Polytechnic Institute and State University
Blacksburg, Va. 24061

Recent work has been on two tasks - droplet size measurements in transverse jets and break-up of particle-laden liquid jets in air.

The droplet size measurement work has involved first refinement of our earlier instrumentation and techniques to improve accuracy and to provide for more routine operation. Systematic testing is now underway with glycerin-water solutions for viscosity variation and alcohol-water solutions for surface tension variations. A supporting test program to carefully document penetration and break-up results at the same test conditions has shown a sensitivity to viscosity variations.

A study of the break-up of solid-particle-laden liquid jets in air has been initiated using glass beads (1-40μ diam.) in water. Techniques for producing and handling such slurries have been developed. The initial test program involved injection into quiescent air for comparison with the classical Rayleigh problem involving pure liquid jets.

TURBULENT MIXING AND COMBUSTION IN HIGH SPEED FLOWS/AFOSR-PO-79-00002

G. D. Smith, T. V. Giel, and C. E. Peters

Sverdrup/ARO, Inc., AEDC Division
Arnold Air Force Station, TN

The objective of this research is the development of reliable and physically perceptive analytical models for the turbulent mixing and heat release mechanisms in turbulent combustion systems. The approach taken in this theoretical and experimental study is to develop analytical models for the particular flow processes, then to conduct detailed experiments in order to verify and refine the models. Major emphasis is placed on the development of adequate models for (1) the turbulent transport properties for momentum, energy and mass in a variety of free and confined mixing systems, including flows with chemical reactions and recirculation, and (2) the interaction of heterogeneous turbulent mixing and finite rate chemical reaction.

During FY79, the experiments on ducted, recirculating hydrogen-air flows, both with and without chemical reactions occurring, in a duct-to-nozzle exit diameter ratio 2.5 configuration were completed. Wall static pressure distributions and radial profiles of total pressure, velocity components, static temperature and gas composition were obtained at six axial locations for a hydrogen/air mass flow ratio of 0.00345. All measurements were made both with and without chemical reactions occurring. The radial distributions of mean axial and mean radial velocity, axial and radial turbulence intensity, and the uv velocity cross correlation were obtained using a two-component Bragg-diffracted laser velocimeter. Gas static temperature and air specie number densities were obtained in the chemically reacting flow field using an in-situ pulsed laser-Raman spectroscopy apparatus. A summary technical report, complete with tabulated data, is currently in publication. The results clearly indicate that the mixing in the chemically reactive flow field is slower than for the nonreactive case and the presence of chemical reactions has a significant effect on the size and location of the recirculation zone within the mixing duct. The maximum turbulence intensities which occurred in the center of the mixing layer and within the recirculation eddy were very high having values in excess of 20 percent of the jet exit velocity. The results indicate that the flow field for the diameter ratio 2.5 configuration is quite different from that of the diameter ratio 10 configuration previously investigated.

The test cell has been modified by blocking the annular passage and providing for injection of propane into the air stream upstream of the sudden expansion, thus providing a premixed hydrocarbon/air

dump combustor configuration. Testing with the modified apparatus has been initiated in FY79 and will continue into FY80.

In FY80, measurements to be made in the flow field, both with and without chemical reaction occurring, will consist of the total pressure field, duct wall static pressure distribution, and radial profiles of the axial, radial and fluctuating velocity components obtained with a two-component, Bragg-diffracted laser velocimeter. Additional flow field mapping of static temperature and specie concentrations will continue into FY81.

Mixing and Combustion in High Speed Air Flows

(F49620-77-C-0044)

R. B. Edelman
P. T. Harsha

Science Applications, Inc.
21133 Victory Boulevard
Canoga Park, California 91303

This project has been concerned with the development of analytical models for high speed combustors, with emphasis on the sudden expansion (dump) combustor. A modular model for the sudden expansion combustor has been developed, which combines empirical and analytical formulations for the major elements of a sudden expansion combustor flowfield. For example, empirical expressions are used to compute fuel penetration and fuel vaporization rates, while analytical models are utilized to determine fuel spread, and subsequently flame propagation rates within the combustor. The analytical modeling of the combustor combines a parabolic solution procedure for the directed flow with a stirred reactor formulation for the recirculation zones; these models are iteratively coupled through their boundary conditions.

During the current period, the modular model has been refined through the use of a two-equation turbulence model and applied to the computation of the premixed combustor flowfield tested by Craig, et al. at AFAPL. Results of this work will be presented. Key conclusions are:

- The recirculation zone state of reaction is an important parameter in the determination of overall combustor performance.
- Mixing characteristics within the combustor are strongly affected by the turbulent intensity and scale within the recirculation zone.

A major focus of effort during this period has been a detailed examination of the processes involved in fuel spray vaporization and combustion. In particular, the effects of fuel volatility and viscosity are being examined; these physical properties can be substantially different for heavy hydrocarbon fuels than for conventional ramjet and turbojet fuels. Results of a study of the effects of the physical properties of fuels with respect to their impact on combustor performance as a function of operating conditions will be discussed.

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Tuesday AM

TUESDAY

AGENDA

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FLAME EFFICIENCY, STABILIZATION AND PERFORMANCE IN PREVAPORIZING/PREMIXING COMBUSTORS
AFOSR-77-3446

A. M. Mellor

The Combustion Laboratory
School of Mechanical Engineering
Purdue University
West Lafayette, Indiana 47907

Advanced combustor design concepts involving fuel prevaporization and premixing upstream of the flame stabilization zone are considered. Applications include automotive, catalytic, ramjet and aircraft propulsion systems. However, problems of poor combustion efficiency and lean blowoff must be overcome. The Purdue research program considers these problems using a simplified sudden expansion combustor, a compromise between the disc flameholder, which has been studied extensively by Tuttle et al. (1977) for EPA, and the dump ramjet burner of Stull et al. (1974). Flame stabilization results from a bluff body recirculation zone characteristic of ramjet and turbojet afterburners.

During the current grant period, preliminary centerline cold-flow LDV measurements were made of the tube and disc geometry and the inlet air stream to the combustion test section. Seeding was provided by oil droplets in the inlet air. Inlet LDV measurements resulting from the uncontrolled seeding appear biased by -8% when compared to pitot tube measurements. No velocity data were obtained for the tube and disc configuration due to insufficient data rates. Doppler signals were seen but were on the order of 10 per second in the flow around the disc. No signals were detected in the recirculation zone, thus verifying the need for direct seeding near the disc surface. In the upcoming year, a dedicated LDV system will be installed at the facility. A complete velocity mapping in both cold and reacting flow will be performed in the wake of the tube and disc. Natural seeding will be augmented by phenolic resin microballoons provided by a fluidized bed seeder. This will also provide seeding in reacting flow. Attempts will be made to identify fuel droplets in reacting flow using the LDV.

Development of the finite difference numerical simulation code "CORA2", made available by D. B. Spalding, was begun. The code is two-dimensional elliptic, gas phase and includes the κ-ε turbulence model. The reaction model is that of a simple chemically reacting system governed by an Arrhenius expression or by the eddy break-up model; the slower is used to estimate heat release rate. Non-reacting flows were modeled for the disc in duct (Tuttle et al., 1977) and the AFOSR tube and disc arrangements. Comparison with LDV will be made. Currently, the start of calculation is at the

plane of the disc. Future efforts include starting the calculation upstream of the tube and disc, specifying inlet velocity profiles, and considering the combustion of a propane/air mixture. Comparison with detailed probings will be made. The data of Tuttle et al. (1976) was recently used by Whitelaw and Banhawy (1979) for comparison with a similar finite difference technique.

The study of classical flashback is now possible at the Purdue test facility as a result of replacing the upstream slave burner with an indirect fired heat exchanger for air preheating. Research to investigate the actual limit for classical flashback will begin in the near future. Adaption of the characteristic time model (Mellor, 1976) will then be made to explain the results.

The detailed probing of flames is still being performed. Diagnostics have been added to better establish boundary conditions for future modeling efforts using CORA2. Following the completion of detailed probing any insight into the flame structure will be applied to the combustion efficiency data of Plee et al. (1977) and an attempt to successfully correlate it will be made.

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TURBULENT VORTEX FLOW-FLAME INTERACTIONS, PROGRAMMED FUEL-AIR EXPLOSION AND COUPLED DROPLET EVAPORATION AND DECOMPOSITION AFOSR GRANT 77-3354

P. Roy Choudhury and Melvin Gerstein

University of Southern California
Department of Mechanical Engineering
Los Angeles, California 90007

There are two major goals of this program. One part deals with the investigation of flow-flame interaction in a swirl burner and the other with the understanding of the inefficiency of the evaporation process of liquid fuels at higher pressures typical of the advanced combustors. The combined results of both parts help the formulation of design guidelines for more efficient advanced propulsion systems.

Inefficiency of droplet evaporation due to liquid phase decomposition can cause a significant reduction in the combustion efficiency of an otherwise efficient burner. As an extension of the evaporation studies, the use of dissolved materials followed by controlled evaporation can be used to provide non-reactive and non-explosive dispersion of free radical generators and explosives, followed by programmed reaction or explosion.

The beneficial effect of swirl generation and vortex amplification by gas jets has been demonstrated for both the small laboratory scale and more realistic larger burners. Also, the flame blowoff results from a small scale burner operating at low pressure and temperature can be used for predicting the lean blowoff performance of larger burners with choked nozzle operating at higher pressure and temperature. Swirl can also be introduced in the flow field by means of mechanical guide vanes which are permanently located upstream of the dump plane. Because of the increase in flame spreading, the use of guide vanes can also increase the combustion efficiency. Experiments performed with hubmounted guide vanes show that the loss of stagnation pressure is higher with the guide vanes than with the air jets. However, the lean blowoff performance of these two different swirl generators are very similar. The primary shortcoming of the mechanical guide vane is the pressure loss which progressively increases with the upstream velocity. The main disadvantage of the swirl jet system is the availability of the bleed air and both thermal and chemical quenching at the injection point.

In the concept of gas-generator ramjet, appropriate swirl can be introduced in the flow field by choosing the angle at which the primary flow enters the burner. A swirl side dump burner is expected to have a high combustion efficiency without the pressure loss associated with mechanical hardware such as guide vanes. A parametric study of the location of the dump planes, their angles, and other characteristics is about to begin. Emphasis will be placed upon the phenomenon of low frequency combustion oscillation and rumble which have been observed in dump burners. For the swirl side dump concept, the fundamental causes and possible remedies of pressure oscillations would be studied.

The inefficiency of droplet evaporation due to liquid phase decomposition at higher pressures results in a nonlinear form of D^2 vs t relationship. Under such a condition, a coupling between evaporation and liquid phase decomposition can cause a large reduction in the combustion efficiency of a burner. Analytical model of coupled liquid phase decomposition and evaporation in a two-phase flow system shows that nonvolatile residue progressively inhibits the evaporation process. In order to avoid the detrimental effect of too much residue formation, one must try to increase the evaporation rate. Larger droplets and longer residence times accompanied by small initial relative velocity between the droplet and the gas should be avoided.

Since the boiling temperature of the liquid increases with increasing pressure, the decomposition rate would also increase with pressure. Therefore, the combustion inefficiency would also tend to increase as the pressure is increased. The aromatics, napthenes, and olefins in the fuel tend to increase the decomposition rate so that for commercial fuels, the fuel composition is a factor in evaporation efficiency. Future fuels, the so-called alternate fuels derived from coal and shale oil, are likely to present major problems related to liquid phase pyrolysis. Slurries also change the local temperature and reaction conditions within the condensed phase and thereby affect the evaporation and combustion efficiency. Therefore, in addition to reducing combustion efficiency, liquid phase pyrolysis can cause excessive carbon deposit and soot and particulate formation.

AFAPL Supported Research Development Trends and Needs in Aircraft Fire and Explosion Technology

J. R. Manheim, B. P. Botteri
Air Force Aero Propulsion Laboratory (AFAPL/SFF)

Abstract not received

AFFDL SUPPORTED RESEARCH, DEVELOPMENT TRENDS AND RESEARCH NEEDS ASSOCIATED WITH AIRCRAFT FIRES

R. Lauzzy, C. Anderson
AFFDL/FES

Abstract not received

GENERATION OF FUEL MIST BY PROJECTILE PENETRATION
F33615-77-C-2069 Task 35

Lee A. Cross and Stephan J. Bless

University of Dayton Research Institute
Dayton, Ohio 45469

This work concerns splash and spray from high speed projectiles exiting through liquid free surfaces. The principal motivation for the investigation derives from a problem in aircraft survivability. Projectiles which penetrate fuel tanks may produce spray in the ullage and the fuel/air mixture in the ullage may become combustible. If the projectile is an incendiary, a catastrophic fire or explosion may occur.

The combustion properties of a flammable liquid/air mixture are chiefly determined by the liquid drop size distribution and number density. Therefore, we have carried out a preliminary definition of experimental and theoretical approaches which might be applied to predicting drop size and density as a function of position and time in such encounters. Two diagnostic procedures: high framing rate photography (up to 6000 fps) and laser-illuminated still photography have been employed to analyse the morphology of the splash produced when a projectile enters the bottom of a shallow water vessel and exits through its' upper free surface. A special upward-firing vertical range with a 0.30 caliber barrel was employed to launch conventional lead-nosed bullets at a velocity of 720 m/s.

Photographs recorded with the high framing rate camera in conjunction with the laser-illuminated photographs have clearly illustrated the mode of evolution of the splash dome and the very fine mist generated by a projectile impact on the lower surface of the fluid. The following sequence of steps is believed to represent an accurate description of the sequence of events following the impact of a projectile with the bottom of the water container:

(1) As a projectile enters the water, a cavity is formed surrounding the projectile which is filled with air and water droplets on its periphery. This cavity continuously grows laterally in size until all the water is fragmented, at least in the small diameter containers which were employed in this study. The concentration and size of the droplets which may be present in the cavity could not be determined by the photographic methods which we employed.

(2) The flow induced by the projectile results in the continuous water being lofted upwards and outwards. The exact timing between impact and the rise of the dome was not determined. However, it was established that over the distance which the splash was observed (∿30 cm), the projectile does not break out of the splash.

(3) The formation of minute droplets (mist) that are too small to be photographically recorded occurs within 100 μsec of the time when the dome begins to rise. No evidence exists that large drops form which subsequently break up into smaller and smaller droplets. From the very earliest laser-illuminated photographs, the top of the dome is either continuous (before the dome has risen any appreciable distance) or consists of droplets which are too small to be photographed.

(4) As time proceeds further, the very fine droplets continue to move upward at a very high velocity (approaching or exceeding that of the projectile) and the remaining continuous water continues to expand, moving rapidly upwards and slowly outwards at the top and slowly outwards at the sides. As the continuous water on the upper sides rises and expands, surface instabilities begin to appear as protuberances and irregularities in the previously smooth surface. These instabilities appear first close to the position where the fragmented and continuous water join and then appear further and further down the water column as time proceeds. These instabilities are probably of the Rayleigh-Taylor or Helmholtz type. As the surface breaks up, large drops (>100μ) are formed, but apparently not in great quantities and, in fact, they may be slowed by aerodynamic drag so much that the continuous water catches them again.

(5) Although the evidence for this is weak, it is believed that the fine droplets at the top of the dome are subjected to tremendous deceleration forces due to aerodynamic drag. Preliminary estimates based on fragmentary data indicate that the deceleration rate may be as high as $7.7 \times 10^5 g$.

(6) There is evidence, based on the laser-illuminated photographs in which motion blur is negligible, that certain types of instabilities may affect the upper portion of the splash dome also. The nature of these is presently unknown, but evidence for them exists due to the presence of irregular, large protuberances in the fine droplet cloud near the top of the dome. These could be formed by projectile fragmentation or by large aerodynamic instabilities due to the passage of a large amount of supersonic water through the air above the water containment vessel.

The general evolution of the dome was shown to be reproducible in the main but the two types of irregularities: those on the continuous water surface and the large protuberances on the upper dome, are not. Changing the water from ordinary tap water to water heavily doped with Photoflo to reduce its surface tension produced no discernable changes in the dome evolution except that the surface instabilities appearing on the lower continuous water surface seem to be more prevalent in the case of the water with Photoflo.

No definitive photographs containing evidence for small water droplets were obtained. It was demonstrated that clear photographs of fibers could be produced for fibers as small as 20 microns, but an extensive search of the upper splash dome in more than 20 negatives showed that no droplets could be seen. The evidence indicates that droplets as small as 4 - 5 microns should have been detectable.

The instabilities which appear on the continuous water of the lower dome do produce drops of a size which can be recorded photographically. However, these are probably not of as great an importance in producing an inflammable vapor cloud as the small droplets in the upper dome. They are so large that a considerable breakup of these drops would be necessary before they become small enough to contribute appreciably to the vapor concentration. They each contain a large mass of fluid, however, and if secondary breakup due to impact with the walls of the fuel tank are important, they could contribute an important source of small droplets.

ABSTRACT

1979 AFOSR Contractors Meeting
on
Airbreathing Combustion Dynamics and Kinetics

MULTIPLE IGNITION, COMBUSTION AND QUENCHING
OF HYDROCARBON FUEL SPRAY

Contract No. AFOSR-76-3052

William A. Sirignano, Principal Investigator

Carnegie-Mellon University
Schenley Park
Pittsburgh, Pennsylvania 15213

The ignition of combustible gas mixtures by burning metal particles (sparks) presents a safety problem in several areas. It is the mechanism by which incendiary weapons are effective and also has been studied as a source of ignition during aircraft crashes. Also, it is a major cause of explosion in coal mines. A joint experimental-theoretical program for the study of this ignition process has been initiated at Princeton University and recently moved to Carnegie-Mellon University with the principal investigator.

Aluminum particles of varying diameter (20μm to 80μm) were suspended on a glass fiber in a methane/air or propane/air combustible gas mixture at room temperature and pressure. The particle was heated and caused to burn by a pulse from a Nd: Glass laser. The minimum diameter of single burning aluminum particles that ignite methane/air mixtures was determined experimentally to be between 20μm and 30μm. The minimum diameter is less than 20μm for propane/air mixtures and is presented as a function of fuel/air equivalence ratio, ϕ. The energy of combustion of aluminum particles of minimum diameter (0.3 to 1.0 mJ) is of the same order as the minimum spark ignition energy of the gas. The methane/air mixture ignitable by the smallest particles has about the same equivalence ratio ($\phi \sim 0.9$) as the mixture ignitable by the least energetic spark; and the propane/air mixture ignitable by the smallest particles has an equivalence ratio ($\phi \sim 1.5$) greater than the mixture ignitable by the least energetic spark ($\phi \sim 1.25$). This was unexpected because the burning aluminum removes oxygen from the combustible gas making the mixture fuel-rich in the vicinity of the particle. Data from the present study and two previous studies verify that, among various metals, the minimum particle mass for ignition of the gas is inversely related to its heat of combustion.

The experimental results for methane-air mixtures were reported in detail at the last Western States Section/Combustion Institute Meeting by Homan and Sirignano. A paper reporting both methane-air and propane-air results has just been submitted for archival publication.

Numerical predictions of ignition by hot, inert particle do indicate that a minimum size for ignition does exist. Also fuel-air mixture ratio affects ignition through the chemical rate. These finite-difference transient calculations will be published shortly by Su, Homan, and Sirignano in Combustion Science and Technology. More recent theoretical work involves a second-order perturbation approach to the problem.

In particular, the method of matched asymptotic expansions is applied for the study of the ignition of a combustible mixture by an inert particle via steady-state analysis. The activation energy is assumed to be large, and the inverse of a reduced activation energy β is taken so the perturbation parameter. A critical Damkohler number (a minimum value for ignition to occur) is found through order β. This second-order solution is in better agreement with our numerical calculation of the transient case than the first-order solution of the steady case by Law.

Future plans include extension of the experimental program to: (1) study non-aluminum particles with methane-air mixtures and (2) study aluminum particles with liquid fuel-air sprays. The theoretical study will be extended to include the effects of: (1) burning metal particles and (2) heterogeneous hydrocarbon combustion.

THE PREVENTION OF AIRCRAFT FIRES FROM FUEL LEAKS IN FLIGHT AND IN GROUND CRASHES

Robert L. Altman
NASA-AMES Research Center
Moffett Field, California 94035

A. New Dry Chemicals for Extinguishing Jet Engine Nacelle Fires

When fuels leak onto surfaces of an operating engine they can ignite when engine case temperatures exceed 1010°F (565°C). As aircraft are redesigned to fly at higher mach numbers the engine case temperature, the bleed air temperature, the maximum air velocity, and the fire extinguishment storage temperature requirements all increase making the task of extinguishing fuel-leak fires more difficult. We have undertaken to find new fire extinguishments more effective than the CF_3BR, CF_2BR_2, and CF_2ClBR in current use. Besides testing commercially available dry chemicals our research endeavor has been to develop and test new dry powder fire extinguishants which when discharged into a fire scene resembling a jet engine fuel leak fire stick to hot surfaces and after putting out the initial fire act as an anti-reignition catalyst even when the fuel continues to leak onto the heated surface. (This program was sponsored by WPAFB with military interagency purchase requests FY 145575-00511, 145576-00617, and 145578-00624 and the research carried out at Ames Research Center with the assistance of Professors A. C. Ling, L. A. Mayer, and D. J. Myronuk of San Jose State University.)

B. Role of Drag Reduction in the Development of Anti-Misting Kerosene

Jet fuel may yield fine droplets upon forced discharge from a fuel tank which has ruptured in a ground crash and elimination of these droplets can reduce the incidence of post-crash fires. To achieve this goal, "Anti-Misting kerosene" which is a fuel like jet-A or JP-5 with less than 1% dissolved polymer additives all exhibit significant drag reduction when dissolved in jet fuel. We have been investigating the relationship of drag reduction to anti-misting effectiveness by making a photographis study of jet fuel dispersions with and without such additives. (This initial investigation was sponsored by NASA-Ames Research Center with defense purchase request A-59059B and the photographic jet study was performed by Dr. J.W. Hoyt and J. J. Taylor at the Naval Ocean Systems Center in San Diego, California.)

Ignition of Fuel Sprays by Hot Surfaces and Stabilization of Aircraft Fires (Contract/Grant AFOSR-77-3446)

J.G. Skifstad and A.H. Lefebvre

School of Mechanical Engineering
Purdue University
West Lafayette, Indiana

This research activity is concerned with two general topics related to aircraft fire safety: (1) the ignition of fuel sprays by hot surfaces and (2) the stabilization of both external and internal aircraft fires. Existing data are insufficient to enable assessment of aircraft fire hazards under the extremely broad range of conditions possible for such hazards. Fundamental experimental data are to be obtained as needed and appropriate theoretical descriptions of the phenomena for hazard assessment purposes are to be developed.

Ignition of fuel sprays by hot surfaces is being investigated in an apparatus wherein a fuel spray is injected into an airflow with known properties and the mixture is passed through a heated length of pipe. The influence of detailed spray, airflow, and surface properties are to be investigated for each fuel considered under a wide range of conditions. The experimental arrangement is described in AFOSR TR-79-0079, and was discussed at some length at last year's meeting. Preliminary runs with the system have shown ignition temperatures to be in the vicinity of 1300°F for low-velocity stoichiometric mixtures of kerosene (JP-4) in air for which the SMD of the fuel spray was in the 50 micron range. Most of the experimental activity this year has been devoted to refinements of the system, tailoring the LDV system to the measurements in these types of sprays, and to the development of a heated probe/analysis system for sampling measurements. The requirements for LDV probe volume, signal conditioning, and the like are to be discussed, along with the computer interface arrangements. A description of the heated sampling probe system and analysis train (CO_2/H_2O) is also to be presented. Comparisons of scattering and imaging measurements of spray properties will be examined as they relate to the methods chosen for the experiments.

Insofar as one of the objects of this investigation is to develop models for the prediction of ignition under rather broad ranges of conditions, an extensive literature search has been made, dealing with all facets of atomization, spray dynamics and transport, and chemical phenomena involving sprays. Several thousand references have been accumulated to that end. While this activity is only partially attributable to funding under the AFOSR Grant, it will be continued and expanded as funds from other sources become available.

Stabilization of aircraft fires by large-scale flameholders is to be investigated in a combustion tunnel initially with V-type and L-type gutters, using the water injection method developed by Lefebvre. A review of the technical aspects of the problem is to be presented, outlining the data required and the range of conditions to be investigated. The laboratory facilities for investigating flame stabilization were redesigned this year to incorporate both a large system (10-inch square test section) and a smaller system (6-inch pipe) for pilot studies. Most of the hardware, controls, fuel system, etc., have either been installed or are in hand. Preliminary runs with the smaller of the systems will be described.

A FEASIBILITY STUDY OF SCALING THE AIRCRAFT EXTERNAL FIRE/F33615-79-C-3420

N. A. Moussa

Arthur D. Little, Inc.

Cambridge, Massachusetts

Combat aircraft are subject to the possibility of a ballistic hit that could rupture the fuel cell. The resulting fuel leakage may then ignite, yielding an in-flight external fire that threatens the aircraft. Combat pilots have reported that, sometimes, they can significantly modify the character of this fire by maneuvering the aircraft. To increase the survivability of an aircraft under these conditions, it is important to determine the effects of the flow field on the fire.

A full-scale study of the aerodynamics of aircraft external fires would be extremely difficult and prohibitively costly. Accordingly, the Flight Dynamics Laboratory, at Wright-Patterson Air Force Base, issued a request for proposal to determine the feasibility of conducting the study on small-scale models. Arthur D. Little, Inc., was awarded this contract in the beginning of fall 1979.

The objective of this program is three fold: first, to determine the scaling laws that must be maintained invariant between model and prototype; secondly, to specify the experimental requirements for testing the scale models; and thirdly, to formulate an experimental plan to test the validity of the scaling laws. In this talk, we will describe our technical approach to these three tasks and any preliminary findings obtained so far. This approach is summarized below.

To determine the scaling laws, we will subdivide the highly complex external fire problem into a number of simpler subproblems that can be treated separately. We will formualte these subproblems along the lines of classical problems that have been treated in the literature, such as fuel input into an airstream, flow field around an airfoil , flame stabilization in a circulation zone, etc. For each of these subproblems, we will identify the involved scaling parameters, and will utilize semi-empirical data from the literature to assess their relative importance. We will then combine the most important scaling parameters to determine the scaling laws that must be maintained invariant between model and prototype.

Based on these scaling laws, we will evaluate various approaches of scale model testing. In each case, we will describe an experiment in which a "control" variable(s) will be modified to maintain similarity for the small-scale model. We will examine the requirements of each experiment in terms of scale model fabrication, operating characteristics of test facility, and instrumentation. We will weigh the feasibility of such requirements against the

anticipated results from each test to select the best testing approach.

Finally, we will develop a testing plan to verify that similarity is maintained between various reduced-scale models according to the proposed scaling laws.

In preparation for the analyses described above, we reviewed the literature for pertinent previous work. Our preliminary findings are summarized below.

Flames are stabilized in boundary layer flows by one of two mechanisms. The first occurs when a flame finds a position where the flow speed equals and opposes the burning speed, and the distance from any quenching surface is greater than or equal to the quenching distance. The second occurs in a region of reversed flow, where hot products of combustion act as a source of continuous ignition of the unburnt mixture. This later mechanism appears to be the predominant one for the conditions of the aircraft external fire.

For flame stabilization in recirculation zones, numerous experimental studies have been conducted behind bluff bodies such as cylinders, spheres, discs and cones. The flammable mixture consisted of either premixed fuel air vapors or a liquid fuel spray injected in the air stream.

Blow off data on such systems have been generally expressed in the form of an inverted U-shaped relationship between a stability parameter and the fuel air equivalence ratio. Various stability parameters have been formulated by various investigators, such as: a ratio of ignition delay time to flow time, a ratio of rate of energy removed by convection to that liberated by chemical reaction, a dimensionless measure of flame stretch due to gradients in the flow velocity, and a dimensional fuel loading parameter. These formulations are presently being reviewed and compared to assess their applicability to the aircraft external fire problem.

The results anticipated from this study will establish the feasibility of utilizing small-scale models to study the aircraft external fire. Should the methodology prove feasible, systematic studies can then be conducted to determine design and operating procedures that would increase aircraft survivability.

Ignition of a Liquid Fuel Under High Intensity Radiation
(AFOSR-ISSA-79-006)

Takashi Kashiwagi
Center for Fire Research
National Bureau of Standards
Washington, D.C.
20234

Laser technology has been rapidly advancing in the last several years. Power outputs of modern lasers have increased significantly and these lasers can now be used as tactical weapons. A high power laser weapon can ignite aircraft fuel tank penetration and can thus cause a fire or explosion on the aircraft. However, the ignition of flammable liquids by laser radiation has been little studies and is little understood. The objective of this study is to obtain a fundamental understanding of the mechanism of ignition of flammable liquids by a high power laser.

An experimental study of the key processes during ignition and a theoritical study of the modeling of a part of the phenomena during the ignition period are being conducted. The experiments were carried out using a CO_2 laser and n-decane as the flammable liquid. High speed pictures by shadowgraph, schlieren and direct method were taken to observe the phenomena of ignition. Shortly after irradition of the decane surface, schlieren pictures show vigorous vaporization. At the same time, direct pictures show the growth of a half-sperical bubble-like depression beneath the surface. This depression grows rapidly to about 3 mm diameter. After a certain period which appears to depend on flux and the incident angle of the incoming laser, the depression starts to collapse and under some conditions the depression disappears completely. After the disappearance of the first depression another depression is formed rapidly. Again, the second depression collapsed and this cycle of the formation of the depression and its collapse is repeated during the ignition period and even after ignition. It is postulated that the surface depression observed during the ignition period is caused by the momentum of the decane vapor leaving the decane surface. The periodic collapse of the depression can be explained by the absorption of the laser beam by the decane vapor in the gas phase; this reduces the laser energy input to the decane. A detailed discussion of the formation of the depression and its periodic collapse will be presented.

A simplified theoretical model to describe the development of a plume in the gas phase was developed as a foundation for a more complete model. Two different approaches are being used in this study, one is numerical and the other is analytical. The analytical approach and some preliminary results will be discussed.

REACTIONS OF HYDROCARBON GASES INITIATED BY A PULSED INFRARED (CO_2) LASER, CONTRACT F 33615-77-C-2004

S. C. Khandelwal, M. D. Porter and G. B. Skinner

Department of Chemistry, Wright State University

Dayton, Ohio 45435

The objective of this program is to study the dissociation and ignition of hydrocarbon fuels in the gas phase caused by irradiation from a pulsed CO_2 laser. Propane was taken as prototype hydrocarbon because it is the simplest paraffin which absorbs appreciably at 10.6 μm. Reaction pressures were relatively high (many of our experiments were at 60 torr) to simulate aircraft fuel tank conditions.

The laser was a Lumonics Model TEA-602, that could emit up to 150 J per pulse, with about half the energy in a 70 nanosecond spike and the balance in a 1 microsecond tail. The energy density in the center of the beam was about 2 J/cm^2 in a pulse, but we could increase this value by focussing with a 100 cm focal length NaCl lens. Samples were irradiated in cylindrical cells fitted with NaCl windows, and products analyzed for by gas chromatography.

Four series of results are reported, as follows:

1. With an unfocussed beam of 2J/cm^2 and NaCl windows on both ends of the cell, no reaction was observed with up to 240 pulses.

2. With an unfocussed 2J/cm^2 beam and an aluminum reflector at the downstream end of the cell so as to double the exposure of the gas, 0.3% reaction was observed in 1 pulse and several percent with 10 pulses. This reflector was not highly polished (1.5 μm rms finish) and we suspected surface-initiated reaction.

3. With similar beam conditions and a highly polished aluminum reflector at the downstream end of the cell, no reaction was observed.

4. In this arrangement a polished convex reflector was placed at the downstream end of the cell, to reflect a converging beam back along the path by which it entered the cell. Many experiments at different fluences up to 12J/cm^2 average, and for both pure propane argon mixtures, were made. At higher energies up to 20% of the propane in a 1% mixture in argon at 60 torr could be dissociated, compared to 1.7% decomposition of pure propane under similar circumstances. Reaction products were CH_4, C_2H_4, C_2H_2, C_2H_6, C_3H_6 and small amounts of C_3H_4. Acetylene yields were generally

larger than in thermal experiments carried out in shock tubes.

We also found that under similar conditions ethane, which has a very low absorption coefficient at 10.6 μm, dissociated to comparable amounts under similar conditions. This indicates a substantial contribution by wall initiated reaction (apparently by interaction of the laser beam with the aluminum reflector). Our present view is that most of the reaction we have seen so far is due to wall effects, and we have been trying to understand the mechanisms involved.

We have recently constructed a new cell which will enable us to use high intensities without using a reflector and also without damaging our windows. We hope that this will enable us to observe reaction under completely homogeneous conditions.

Ignition, Combustion, Detonation and Quenching of Reactive Mixtures

R. EDSE

THE OHIO STATE UNIVERSITY

(AFOSR-78-3604)

To develop an equation which can be used to predict the length which a flame has to traverse through unconfined or confined combustible gas mixtures to form a stable detonation wave (induction distance) several series of experiments have been started to study the effects of initial gas temperature, pressure, and density on the induction distance. Calculations have shown that the amount of energy which is transferred from the burned gas downstream of the wave to a unit volume of the gas at the tail of the detonation wave increases greatly as the initial temperature of the combustible gas mixture is lowered. This energy transfer is also increased very much when the initial pressure is increased. On the other hand the energy transfer in a $H_2 + 1/2\ O_2 + 1.88\ He$ mixture is the same as that in a $H_2 + 1/2\ O_2 + 1.88A^2$ mixture when both mixtures are at the same initial conditions and the energy transfer per unit volume is considered. It is planned to investigate the relationship between the amount of energy which is transferred and the induction distance. Measurements of the flame speeds of hydrogen-oxygen-inert gas mixtures at initial temperatures ranging from that of liquid nitrogen to somewhat above room temperature are in progress. These data are needed to determine the relationship between the deflagration speeds of the various mixtures and the observed induction distances. A nozzle type burner tube having a convergent sine curve contour is used for these measurements because it produces rather straight flame cones even at rather large Reynolds numbers.

Measurements of the quenching distances of methane-air, methane-oxygen, acetylene-air, and hydrogen-air flames with and without coatings of potassium chloride, sodium-bicarbonate, or potassium phosphate on the quenching surfaces showed that these coatings did not alter the quenching distances observed with the untreated surface. It was also observed that for laminar flow the quenching distances of these flames are independent of the linear speed of the unburned gas. Variations of the burner width also did not affect the quenching distances. However, rather significant increases of the quenching distances occurred when the narrow open gaps between the two quenching plates were closed.

Preliminary results from experiments with rapidly flowing combustible gas mixtures through constant area ducts indicate that turbulence reduces the induction distance only slightly.

BASIC INSTABILITY MECHANISMS IN CHEMICALLY REACTING SUBSONIC AND SUPERSONIC FLOWS

(Grant AFOSR-78-3662)

T. Y. Toong

Massachusetts Institute of Technology

Cambridge, Massachusetts 02139

ABSTRACT

The main objective of this research program is to study instability mechanisms basic to many problems involving chemically reacting subsonic and supersonic flows. Such problems include those related to combustion instability, detonation wave initiation, structure and stability, turbulence spectra in reacting flows, initiation and suppression of explosions, etc.

Both theoretical and experimental studies have been conducted to investigate the instability phenomena due to wave-kinetic interactions. In particular, the effect of non-equilibrium exothermic reactions on the amplification of acoustic pressure waves was examined. Substantial amplification was found possible under certain conditions. A linearized theory of acoustic-kinetic interactions was successful in predicting the observed amplification rates[1-5].

Recent experimental results[6] indicated that sound wave amplification may lead to the formation of weak shock waves in short time intervals, thereby introducing both hydrodynamic and chemo-kinetic non-linear effects. Under such conditions, a non-linear model is necessary for predicting the temporal evolution of the wave amplitudes and structure.

Non-Linear Wave-Kinetic Interactions

An exact wave equation was derived[7] for non-equilibrium reacting flows with the objective of identifying the non-linear effects that do not appear in acoustic perturbation problems. An approximate wave equation, that takes into account chemical effects, was then developed for high-frequency weak non-linear waves. The approximate wave equation was numerically integrated to predict the amplification rates of weak shock pulses travelling in reacting mixtures. The effect of reaction activation energy β ($\beta \equiv E_A/RT_o$), thermicity D_{II}, initial shock strength δ_i, and pulse duration on non-linear wave amplification were examined. The results have revealed the following features:

(i) In reacting mixtures of high activation energies (i.e., detonable mixtures), non-linear wave-kinetic coupling results in dramatic increases in wave amplification rates, even at low shock strengths. Furthermore, the amplification rates are enhanced with increased exothermicity, shock strength, and pulse duration. In the latter instance, a threshold value is identified, which varies with initial amplitude level and kinetic parameters. Below this minimum value, the amplification rates would be reduced significantly.

(ii) Chemical reactions of low activation energies are not capable of sustaining weak shock waves. The rate of decay of the shock waves increases progressively at higher shock strengths. Moreover, higher exothermicities may enhance attenuation rather than amplification. Experimental results at shock strengths up to ~ 0.5 ($M \sim 1.2$) in photo-initiated hydrogen-chlorine-argon mixtures[8] indeed confirm the predictions at low activation energies.

Numerical Study of Initiation of Detonation

It is emphasized again that the ultimate objective of this work is to explore the role of wave-kinetic coupling in the inception and sustenance of instabilities in reacting flows, particularly in gaseous detonations. The dramatic shock amplification rates in detonable mixtures, predicted by the non-linear study, suggest a possible mechanism for the onset of transverse waves in the reaction zone of a detonation wave. Although it is generally believed that these transverse waves are essential for the self-sustenance of detonations, a thorough understanding of the unsteady events occurring during the initiation process has not yet been accomplished. In particular, the details of the onset of transverse waves, their subsequent amplification, and most important, the mechanism governing their characteristic spacing (or frequency), remains to be unveiled. Such information will aid considerably in obtaining the necessary requirements of initiation (viz., minimum time and power density).

During the past few months, the study of instabilities involved in detonation initiation has been undertaken. The complete non-linear governing equations are numerically integrated to compute the unsteady flow fields of both one-dimensional and two-dimensional piston-supported detonations.

The results of the one-dimensional computations indicate that the detonation wave strength, under certain conditions, may experience large oscillations, around its steady state value, at definite frequencies. As the degree of overdrive is reduced, the amplitude of the oscillations increases, but the frequency decreases. At the Chapman-Jouget conditions (i.e., no overdrive), the amplitude excursions may become as large as 300% of the steady state value. The unsupported one-dimensional detonation is currently being examined.

Preliminary results of the two-dimensional case demonstrate the rapid amplification of transverse disturbances at the wave front. Work is in progress to determine the characteristic features of two-dimensional detonations.

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Overview of the JANNAF Workshop "Pressure Oscillations in Ramjets"

F. E. C. Culick

California Institute of Technology

The subject workshop was held on 7-8 September at the Naval Postgraduate School, Monterey, California. It was intended to be primarily educational and tutorial, bring together two groups: those involved currently in the development of ramjets and ramrockets, and those who have had experience with pressure oscillations in other airborne propulsion systems.

Because there has historically been little overlap of the two groups, the greater portion of time during the workshop was devoted to informal presentations covering the general areas of programs; full-scale and development tests; laboratory and sub-scale tests; instrumentation and data processing; and related experience in other systems. Subsequent discussions centered on origins and mechanisms for pressure oscillations; analysis; consequences and related phenomena; implications for test programs and design; and recommendations.

This presentation will be primarily a summary of the proceedings of the workshop, with emphasis on basic technical issues and recommendations.

AGENDA

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CATALYTIC COMBUSTION APPLIED TO AIR-BREATHING ENGINES
EPA CONTRACT 68-02-3122

R. M. Kendall and J. P. Kesselring

Acurex Corporation
Energy and Environmental Division
485 Clyde Avenue
Mountain View, California 94042

The catalytic combustor has the potential to minimize aircraft gas turbine engine exhaust emissions as well as to permit the combustion of fuel/air mixtures leaner than the low flammability limit. In order to make use of this great potential, a thorough understanding of the important physical phenomena occurring in a catalytic combustor has helped lead to the concept of the graded cell catalyst system. The graded cell catalyst was then used in model gas turbine hardware testing, showing the steady-state performance of the combustor to have exceptional emission characteristics.

Catalytic combustion in a monolith bed includes the interaction of chemical reactions (surface and gas phase), diffusive heat and mass transport (laminar or turbulent), convection, bed conduction, and radiation. During steady operation, the catalytic combustion process can be described as follows:

- Premixed fuel and air are introduced into the combustor.
- These gases diffuse to the catalyst-coated surface of the combustor and react on the active sites at and within the surface. Near the cell entrance, where most of the gas is at low temperature, gas phase chemical reactions are unimportant.
- At the entrance, heat release is controlled by catalytic wall chemical reactions. This heat is transferred by conduction, radiation, and convection. Further down the channel, where the gas has been preheated to a high temperature, gas phase reactions become active. In this region, fuel is rapidly consumed by a "flame type" phenomenon which controls the amount of unburned hydrocarbon emissions that escape the system.
- Surface reaction products diffuse back to the main flow of gases and are carried downstream.

Under normal operating conditions, wall and gas phase reactions are active and very little unburned hydrocarbon escapes the bed for lean and stoichiometric initial mixture ratios. However, it has been experimentally observed that above a certain mass flow limit, small increases in flowrate cause an abrupt rise in unburned

hydrocarbon emissions. The abruptness of the increase indicates that a "flame type" phenomenon has been extinguished. This condition, called breakthrough, represents an upper mass throughput for low unburned hydrocarbon emissions.

Increasing the mass throughput in a catalytic bed to levels much above the breakthrough point can cause the front of the bed to become cool. It has been experimentally found that small increases in mass throughput, once the front end of the bed has become cool, can cause the cool region to spread downstream. At this point, all wall reactions are extinguished and the entire bed becomes cold. This condition, called blowout, represents the maximum mass throughput for hot bed operation.

As a result of an analytical study, it appeared that a catalytic monolith bed used for the purpose of combustion should use large diameter cells at the front of the bed to prevent blowout, and small diameter cells at the back of the bed to minimize the breakthrough of CO and HC emissions. Therefore, superior combustion performance should be obtained by using the catalyst in a graded cell configuration, with large cells at the front end, small cells at the back end, and perhaps one or more intermediate size cells between.

Over 50 graded cell catalyst systems have been tested at Acurex. The primary objective of these tests was to identify the best combustion catalyst for system application, but catalysts were also tested for high temperature operability, performance at high pressure, and conversion of fuel nitrogen to nitrogen oxides. Screening catalysts were obtained from eight sources, including W. R. Grace and Company, UOP, Inc., William C. Pfefferle (a private consultant), Matthey Bishop, Inc., Johnson Matthey, DuPont, Houdry Division/Air Products and Chemicals, and Acurex Corporation. Substrate materials were either DuPont alumina or Corning zirconia spinel. Washcoats varied from proprietary preparations with high pretest surface area to no washcoat with low pretest surface area. Catalysts were either precious metal, metal oxide, or mixtures. The post-test surface area always shows a significant reduction from the pretest surface area, as does the noble metal dispersion.

Catalysts were aged for 10 hours and compared in maximum throughput, varying stoichiometry, and minimum preheat tests. Most catalysts were tested in a complete 20 to 30 hour test sequence. Both noble metal and metal oxide catalysts have been tested with extremely high volumetric heat release rates (to as high as 1.08×10^6 kW/m^3-atm) and low emissions.

While many graded cell catalyst systems had been successfully tested over a range of operating conditions, a definitive test comparing the performance of a graded cell system and a single

cell system of identical catalyst composition had not been carried out. To accomplish this test, two catalyst configurations were supplied by UOP, Inc. on DuPont Torvex alumina honeycomb. The graded cell system consisted of three 2.54 cm segments with cell sizes of 6.4 mm, 4.8 mm, and 3.2 mm. The single cell system used three 2.54 cm segments with 3.2 mm cell size. Both systems were washcoated and catalyzed by UOP with a proprietary catalyst, and operated in an identical manner during testing, including 5 hours of steady-state operation under lean conditions at 1560K (2350°F) temperature, followed by maximum throughput testing. As a result of this testing, the following was noted:

- At a standard heat release rate of 29.3 kW, emissions from the graded cell and the single cell monoliths were approximately the same.
- Volumetric heat release at maximum throughput for the graded cell was almost three times higher than for the single cell system (2.06×10^5 kW/m^3-atm vs. 0.71×10^5 kW/m^3-atm).
- Under fuel-rich conditions, both reactor types maintained combustion at preheat temperatures as low as 120°F. However, hydrocarbon emissions from the single cell configuration were an order of magnitude higher than for the graded cell catalyst.
- At the standard heat release rate of 29.3 kW, the graded catalyst had a much more uniform axial temperature profile than the single cell system.

This latter point is of considerable importance. In order to avoid possible poisoning effects, the catalyst bed should operate at as high a temperature as possible throughout its length. The single cell reactor runs a significant risk of being poisoned, while the graded cell reactor has a high, uniform temperature profile.

As a result of the graded cell catalyst testing, significant improvements in catalyst performance and maximum catalyst throughput have been noted. Further work on catalyst development is ongoing, including fuel nitrogen conversion testing, pressure operation, and catalyst life testing in both cyclic and extended durability conditions. As improved catalysts are developed, they are used in the system concept testing phase of the program.

A model gas turbine combustor can was designed and tested to demonstrate steady-state combustion characteristics suitable for turbine applications. The model included:

- 293 kW (10^6 Btu/hr) calculated heat release
- Fuel injection of both clean gaseous and distillate oil fuels

- Operation at pressures to 10 atmospheres
- 1367K to 1589K (2000°F to 2400°F) exhaust gas temperature
- Graded cell catalyst element

This system used a multiple conical tube fuel injector similar to a concept developed at NASA Lewis Research Center for the automotive catalytic combustion gas turbine program. In this concept, incoming air entered the apex end of the cones at high velocity where the fuel was injected. The fuel mixed with the airstream as it expanded through the cones and was then injected as a uniformly premixed stream into the combustor. Gaseous fuel tubes injected axially into the center of the cone inlet, while smaller fuel tubes were used to inject diesel fuel normal to the incoming air for vaporization and mixing.

The model gas turbine combustor was first checked out at Acurex with propane between 1.16 and 3.42 atm pressures. Additional testing was conducted at Pratt and Whitney Aircraft in West Palm Beach, Florida at pressures ranging from 2.96 atm to 10.04 atm with propane, No. 2 oil, and No. 2 oil doped with 0.5 weight percent nitrogen as pyridine (C_5H_5N).

Initial Acurex testing was conducted at a 73 kW (250,000 Btu/hr) heat release rate and 1478K (2200°F) bed temperature. No unburned combustibles were measured at any test pressure, and NO_x emissions were less than 2 ppmv at 15 percent excess oxygen. Both fuel injection system and catalyst performed well during the test sequence.

At Pratt and Whitney, heat release rates to 234 kW (800,000 Btu/hr) were achieved with low NO_x emissions for both propane and No. 2 oil. Some difficulty was encountered with flashback and flameholding on the fuel nozzles when running No. 2 oil. High CO and unburned hydrocarbon emissions resulted from operating at low bed temperatures to avoid flameholding. Variations in pressure were not found to affect emissions levels.

The model gas turbine was successful in demonstrating controlled steady-state exhaust temperatures compatible with present turbine machinery. Also, relatively large volumetric heat release rates were obtained, showing that the catalytic combustor can be comparable in size to existing combustors with the same heat release rate. The small volume model combustor further exhibited low overall pressure drop (less than 1 percent at 3 atm pressure), an important factor to turbine system efficiency. The only problem effecting system performance was the tendency of the fuel injection cones to hold flame under some operating conditions with distillate fuel.

HIGH TEMPERATURE CATALYTIC COMBUSTION/ AFOSR-76-3052

P. M. Walsh, C. Bruno, D. A. Santavicca,
B. Kim, and F. V. Bracco

Department of Mechanical and Aerospace Engineering
Princeton University
Princeton, NJ 08544

The objective of this research is to identify the relative importance of homogeneous and heterogeneous kinetics and transport processes in high temperature catalytic combustion and to formulate and test realistic analytical representations of them. Thus this research will contribute to establishing guidelines and techniques for efficient and stable jet engine catalytic combustors and afterburners. Experimental measurements of substrate temperature and gas composition, pressure, and temperature inside and downstream of a honeycomb catalyst are made and compared with the corresponding results from a two-dimensional model. Theoretical and experimental data relative to the oxidation of propane-air mixtures in a platinum-alumina-cordierite honeycomb catalyst are here discussed.

The test rig uses a 25x25x76 mm catalyst sample. Gaseous fuel is injected through a grid of 25 holes and mixed by baffles to achieve ± 1% composition uniformity across the inlet gas stream. The test section is insulated to maintain temperature uniformity of ± 1%. Gas velocity is uniform within ± 6% over the center half of the width of the test section. Substrate temperatures are measured with thermocouples embedded in sealed monolith cells. Gas samples are extracted through a water-cooled probe which contains a thermocouple for simultaneous gas temperature measurements.

Measurements have been made of the lean combustion of propane-air on a platinum-alumina-cordierite honeycomb catalyst at atmospheric pressure, gas velocities of 6-24 m/s equivalence ratios of 0.19-0.32, and inlet temperatures of 650-800 K.

The model consists of the two-dimensional, steady conservation equations for reactive gases in a channel of the honeycomb. The independent variables are the distances along the channel and from the channel axis to the catalytic wall. Thus the structure of the mass, momentum, and energy boundary layers inside each channel is computed. The surface reactions are accounted for as part of the wall boundary conditions and couple

the gas processes to the heat transfer along the solid catalyst which is represented by an ordinary differential equation with the distance along the channel as the independent variable. The model can consider general elementary homogeneous and heterogeneous reactions but the reactions and their constants must be specified. Both laminar and turbulence flows can be computed, the latter via the k-ϵ sub model for the turbulence energy and its rate of dissipation.

In the specific application of the model to the catalytic combustion of propane-air mixtures, the quantities used in comparing measured and computed results were the pressure loss across the catalyst, and the amounts of unburned fuel, CO, CO_2, and O_2 at the catalyst exit versus equivalence ratio, inlet velocity and inlet temperature. The agreement is judged adequate both in trends and values. But such adequacy is not obtained if infinitely fast surface rates or one- or two-step overall homogeneous reactions are assumed. The simplest sufficient model requires finite rate surface reactions and a three-step homogeneous mechanism and show a complex interaction among diffusion, homogeneous reactions, and heterogeneous reactions with none of the three processes being either dominant or negligible.

CATALYTIC FLAME STABILIZATION

Contract No. F49620-77-C-0085

M. Lavid, A. E. Cerkanowicz, W. S. Blazowski

Exxon Research and Engineering Company
Corporate Research-Technology Feasibility Center
Linden, New Jersey 07036

Recent combustion research has identified a number of potentially promising techniques for rectifying the combustion associated aircraft limitations. One of these techniques involves the utilization of heterogeneous catalysis to enhance combustion processes and to broaden normally encountered stability limits, particularly at fuel lean, low temperature conditions. Aeropropulsion combustors would benefit substantially by the improved combustion stability as well as by the increased design flexibility for alternate fuel usage. Primary emphasis in this program is the utilization of the catalytic flame stabilization process in aircraft afterburner systems.

Catalytic combustion is a concept wherein combustion reactions initiated by a heterogeneous catalyst (catalytically active surface) play an important role in the energy release processes of a reacting fuel-air system. It has been demonstrated that a solid catalyst can be used in a manner which provides stable and efficient combustion outside of normal gas phase flammability limits. The catalytic effect is usually dominant only during the early phases of the overall combustion process; as fuel is oxidized and energy is released, the importance of homogeneous reactions increases and eventually these gas phase processes become controlling. For many applications, the key role of the catalyst is to "bootstrap" the conditions of temperature and concentration of partially oxidized reactive fuel species to levels favorable to stable, efficient gas phase combustion. Consequently, a catalytic flame stabilization device need only process a portion of the reactant mixture and need only provide for the initial "ignition" phase of the overall reaction.

The objectives of the catalytic flame stabilization program are to develop a fundamental understanding of the aerothermochemistry of catalytic flame stabilization and to establish design aids to be used in development efforts. Fundamental areas which will be addressed include:

- characterization of the flow field about a catalytic stabilizer.
- determination of the role of the catalyst in stabilizing the combustion process.
- establishment of catalyst and monolith material choices.

- characterization of downstream combustion zone processes (including wake recirculation, turbulent shear layer combustion, and downstream flame propagation).

- quantification of stability limits.

- development of an analytical model of the catalytic flame stabilization process.

The experimental program involves detailed study of the region about various flame stabilization devices. Initially, V-gutter type flameholders and monoliths which are not catalytically treated will be tested to establish an experimental system baseline. Subsequent tests will employ catalytic monoliths or specially fabricated flameholders which simulate catalytic stabilizing device operation. In this latter case, a flameholder with its downstream side sealed with a sintered metal plate will be used. Various gas compositions representing the initial as well as partially oxidized fuels will be passed into the flameholder and through the sintered plate to simulate different modes of stabilizer operation. The temperature of these gases will be varied to evaluate the thermal effect of catalytic stabilization.

Broad variations in catalyst and monolith types will be examined. Catalysts can be prepared from either various noble metals (especially platinum and paladium) singly or in combination or transition metal oxides (oxides of nickel, chromium, etc.). Substrates of different blockage ratios, configuration (triangles, rectangular, circular, etc.), material composition (ceramic or metal), and overall shape (i.e., triangular, disc-shaped, etc.) will be examined.

Fuel-air supply and preparation systems, test section, exhaust system, and basic instrumentation are currently under construction. Test section conditions will encompass the following parametric ranges:

Area:	12.5 cm square or 15.0 cm round
Velocity:	0-200 m/s
Temperature:	300-1000 K (vitiated)
Pressure:	100 kPa
Fuel Type:	liquid or gaseous

Physical probes will be used for pressure and temperature measurement, and for gas sampling. Schlieren photography will be utilized for overall flow field visualization. All data gathering instrumentation are computer interfaced.

Experimental direction and guidance is being provided by a complementary analytical modeling effort. The model is being developed by combining

the existing Exxon catalytic combustor model with bluff body flame stabilization analyses presently available in the combustion literature. Salient features of the physics and chemistry (i.e., aerothermochemistry) of the catalytic mechanism, monolith gas dynamics, wake recirculation, shear layer turbulent reaction, and downstream flame propagation are included in the analysis.

INTERFACIAL CHEMICAL REACTIONS IN FLOW SYSTEMS

Contract F49620-76-C-0020

Daniel E. Rosner[1]

Yale University, High Temperature Chemical Reaction Engineering Laboratory, New Haven, CT 06520

Materials technologies for combustion chambers, heat shields, nozzles and turbine blades, require both theoretical understanding and reliable experimental data on basic gas-solid reactions at high temperatures and laws governing energy/mass exchange with the surface. Our objective is to provide systems and materials engineers with such theoretical understanding and fundamental data on interfacial rate processes, both for gas-surface and gas-particle interactions. Our approach is an interdisciplinary one which draws heavily on experimental results from a class of novel flow reactors. These chemical reactors have been developed for systematic studies of interfacial chemical kinetics, mass transport and energy accommodation under well-defined conditions to facilitate theoretical interpretation.

As typical results of our ongoing AFOSR-sponsored research program on interfacial chemical reactions in flow systems we have:

a) developed a new reactor configuration and data reduction procedures and obtained experimental results[2] for the thermal and chemical energy accommodation coefficients (α, β) and reaction probability, γ, for hydrazine vapor decomposition on platinum and iridium filaments under vacuum flow conditions;

b) developed, extended and applied a new "pseudo-blowing/source" correlation[3,4] for the effects of thermal (Soret) diffusion and variable fluid properties on mass transfer rates in forced convection situations of interest in the fields of soot and chemical vapor deposition (CVD), partial vapor condensation, and surface-catalyzed combustion;

c) developed and applied optical interference and atomic emission (chemiluminescent) techniques to follow the rate of gasification of high temperature surfaces (e.g., $Cr_2O_3(s)$ in the presence of atomic oxygen).

Focusing for the present on topic a, we note that the fate of the energy release in highly exoergic surface-catalyzed chemical reactions is not only of considerable fundamental interest, but also influences catalyst volatilization/sintering, the aerodynamic

heating of hypersonic glide vehicles subject to bombardment by atomic nitrogen and atomic oxygen, etc. To provide the first available high temperature data (T > 800K) on what fraction (β) of the equilibrium reaction energy is delivered to the catalyst per reaction event, two filament flow reactors (FFR) have been developed, well suited to both precise mass balance and isothermal calorimetric measurements. We have published our experimental results[5] for the chemical energy a-commodation (CEA) coefficient β, and the corresponding reaction probabilities, γ, for N-atom association on the metals Pt, Ir, Rh, Pd, Co, W, and Re at temperatures up to 2600K. These measurements have now been extended to hydrazine vapor decomposition on Pt, Ir and W, and in addition to β and γ measurements, we have also experimentally determined the physical energy accommodation coefficient of unreacted N_2H_4.

Our recent results for N_2H_4 decomposition on the noble metals (see Fig. 1) reveal that up to ca. 40 per cent of the prevailing equilibrium decomposition energy can escape the catalyst, however, at catalyst surface temperatures high enough to render the overall (cold reactant, hot product) reaction endoergic, catalyst energy removal is that expected from the equilibrium endoergicity. We conclude with a discussion of the theoretical and practical implications of this line of research, as well as a summary of our plans fo r direct measurements of the excitation energy states of desorbed product molecules.

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[1]Professor of Chemical Engineering and Applied Science, Yale University.

[2]Halpern, B., Kiela, J., and Rosner, D. E. "Energy Transfer in Simple-Surface-Catalyzed Reactions," invited paper (40c), presented at the AIChE 72nd Annual Meeting, 27 November 1979; San Francisco, California.

[3]Rosner, D. E. "Thermal (Soret) Diffusion Effects on Interfacial Mass Transport Rates," J. Physicochemical Hydrodynamics (Pergamon Press, New York), (in press, 1980).

[4]Srivastava, R. and Rosner, D. E. "A New Approach to the Correlation of Boundary Layer Mass Transfer with Thermal Diffusion and/or Variable Properties," Int. J. Heat Mass Transfer (in press, 1979).

[5]Halpern, B. and Rsoner, D. E. "Chemical Energy Accommodation at Catalyst Surfaces: Flow Reactor Studies of the Association of Nitrogen Atoms on Metals at High Temperatures," J. Chem. Soc. (London) Faraday Transactions I. Physical Chemistry, 74, 1883-1912 (1978).

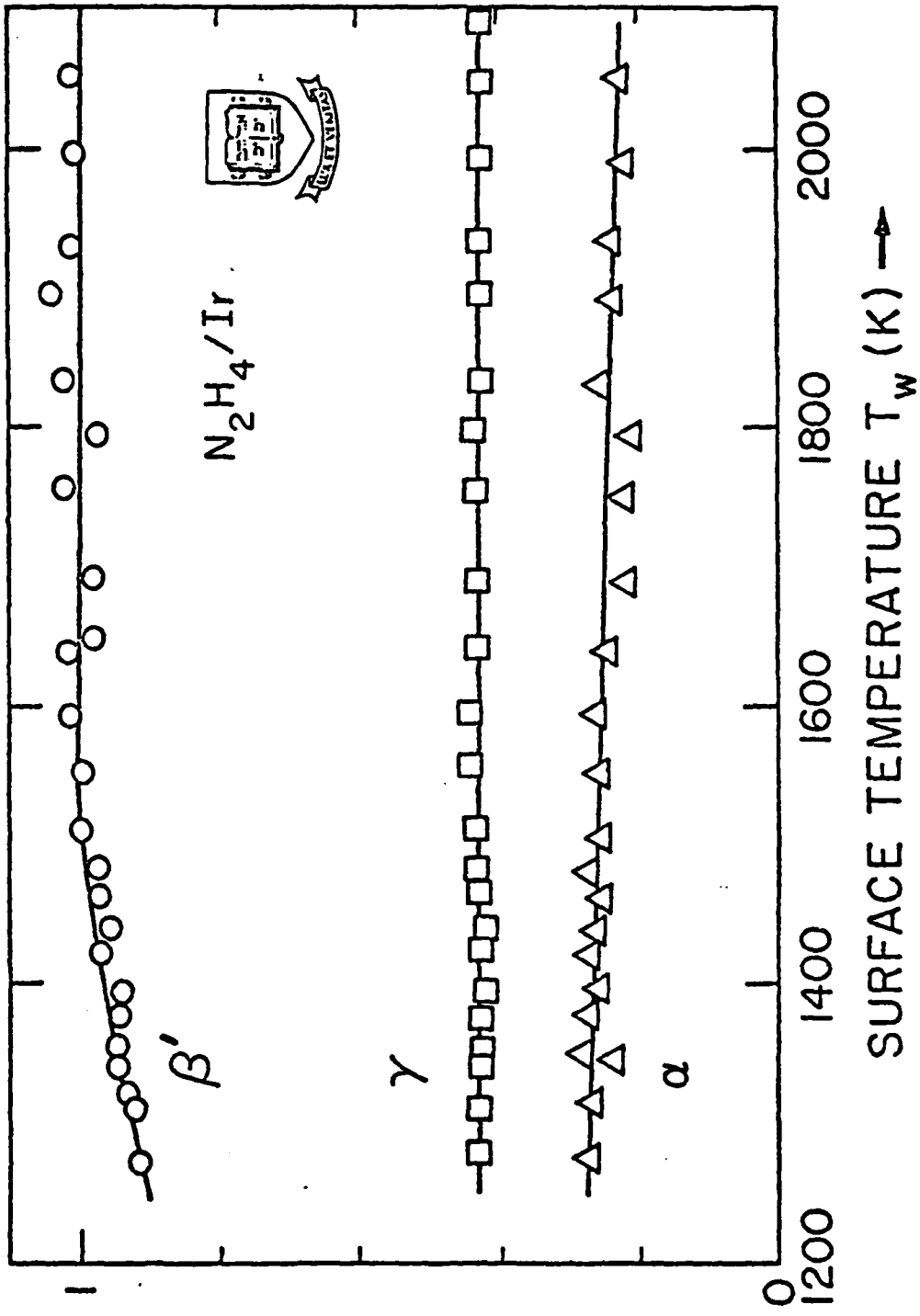


Fig. 1. Chemical kinetics and energetics of the interaction of hydrazine vapor with iridium surfaces at high temperatures; $\beta^1 \equiv$ fraction of 298K exo-ergicity delivered to catalyst, $\gamma \equiv$ decomposition probability, $\alpha \equiv$ thermal energy accommodation coefficient for unreacted N_2H_4 (see Ref. 2).

Utilization of Fundamental Principles and Field Tests to Optimize Combustor Performance and Minimize Exhaust Pollutants

J. Kliegel, S. Hersh, K. Hunter

KVB Engineering Research - Cottrell

Abstract not received

THERMODYNAMICS OF ORGANIC COMPOUNDS
CONTRACT NO. AFOSR-ISSA-79-0007

William D. Good

Bartlesville Energy Technology Center
Department of Energy
Bartlesville, Oklahoma

The Thermodynamics Research Branch of the Division of Processing and Thermodynamics Research at the Bartlesville Energy Technology Center, Department of Energy, is engaged in a continuing program of both applied and basic research on the thermodynamic properties of fuels and of organic compounds that may be useful in the synthesis and development of high-energy fuels. The research group has the skills and equipment needed for combustion calorimetry, heat capacity calorimetry, solution and adsorption calorimetry, molecular spectroscopy, pressure-volume-temperature measurements, measurement of the velocity of sound in compressed fluids, and vapor-pressure measurements. The expertise in combustion calorimetry and vapor-pressure measurement has been utilized in recent years to evaluate both fuels and compounds that have good energy characteristics per unit volume or per unit mass. This investigation has been funded by the Air Force Office of Scientific Research. Earlier research for AFOSR investigated thermodynamic properties of elemental boron and boron compounds, elemental silicon and silicon compounds, organic nitrogen compounds, fluorocarbons, and the organic difluoroamines.

1. COMBUSTION CALORIMETRY OF RJ-6

One of the more recent endeavors of the combustion calorimetry laboratory was measurement of the enthalpy of combustion of RJ-6. RJ-6 is a blend of *exo*-tetrahydrodicyclopentadiene and the hydrogenated dimers of norbornadiene. The material was supplied by Herbert T. Lander, Jr., Fuels and Lubrication Division, Air Force Aero Propulsion Laboratory (AFSC) Wright-Patterson Air Force Base, Ohio. It was used as received without further drying. Fragile flexible ampoules of borosilicate glass confined the samples of RJ-6; auxiliary oil (laboratory designation TKL 66) was used to initiate the combustion. Rotating-bomb calorimeter BMR II and platinum-lined bomb PT-3b were used without bomb rotation. For each experiment, 1 cm^3 of water was added to the bomb, and the bomb was flushed and charged to 30 atm with pure oxygen; nitric acid formation during the combustion was negligible. Each

experiment was started at 296.15 K, and because the masses of combustibles were properly chosen, the final temperatures were very nearly 298.15 K. Temperatures were measured by quartz crystal thermometry; the quartz thermometer was calibrated with a platinum resistance thermometer. A programmable desktop calculator was used to control the combustion experiments and record the results. Readings were taken at 100-second intervals throughout the experiment; integration of the time-temperature curve is inherent in the quartz thermometer reading. The results are summarized in Table 1. The values of $\Delta E_c^\circ/M$ refers to the reaction of unit mass of sample. Carbon dioxide was recovered from all of the experiments. The ratio of carbon dioxide recovered to mass of sample burned was 3.2725 ± 0.0002 (mean and standard deviation of the mean). The empirical formula of RJ-6 calculated from this ratio and the assumption that only carbon and hydrogen are present is $CH_{1.4259}$.

The enthalpy of combustion given in Table 1 is the "gross" heat of combustion for which the reaction products are gaseous carbon dioxide and liquid water. For combustion to gaseous carbon dioxide and gaseous water, the "net" heat of combustion of RJ-6 is -(17971.8 ± 0.4) Btu/lb.

2. HEAT CAPACITY OF RJ-6

The heat capacity of RJ-6 was measured by differential scanning calorimetry in the range 260 to 340 K. The following linear expression was selected to fit the data by means of a least squares fit:

$$C_s = 0.0852880 + 0.000894\,8\ T \text{ cal g}^{-1} \text{ deg}^{-1}.$$

Root-mean-square deviation of results was 0.0055 cal g^{-1} deg^{-1}.

3. VAPOR PRESSURE OF JP-10

The vapor pressure of JP-10 was investigated by inclined-piston-gauge manometry. The initial expectation was that the sample supplied was substantially pure *exo*-tetrahydrodicyclopentadiene, and that the measurements could be done as for a pure chemical compound. That expectation was not realized.

As the measurements are conducted, before each data point is obtained a small amount of the sample is pumped off to flush out traces of permanent gases that could come from slow out-gassing of components of the system. For a single-component sample, the pumping does not change the composition nor the vapor pressure. However, for a mixture of a major component with impurities of different

volatility, the pumping tends to deplete the sample of more volatile impurities and concentrate the less volatile impurities with an attendant decrease of the vapor pressure.

With the JP-10 sample, repeat measurements at a given temperature always showed a lower vapor pressure than had been observed earlier. The last determination was made at 278.15 K and showed the vapor pressure to be only 57 percent of that observed early in the study at that same temperature.

All of the data obtained are shown graphically in Figure 1, with the sequence in which the data points were obtained. These data at least show the general magnitude of the vapor pressure of JP-10 over a temperature range on each side of room temperature, even if they are not suitable for representing by an empirical equation or assigning precise numerical values.

4. COMBUSTION CALORIMETRY OF HYDROGENATED DIMERS OF NORBORNADIENE AND TETRAHYDRODICYCLOPENTADIENE

Experimental measurements are in progress of the enthalpies of combustion of hexacyclic *exo,exo*-dihydrodinorbornadiene and hexacyclic *endo,endo*-dihydrodinorbornadiene and of a newly purified sample of tetrahydrodicyclopentadiene. All of these materials were supplied by Professor C. Moynihan of Catholic University of America.

5. SYNTHESIS AND PURIFICATION OF ALKYLNAPHTHALENES AND ALKYLINDANS

Synthesis and purification of the alkylnaphthalenes and alkylindans with high steric interaction energies continue in the laboratories of Professor E. J. Eisenbraun at Oklahoma State University. Current emphasis is on the alkylindans.

TABLE 1. Summary of Calorimetric Experiments with RJ-6 at 298.15 K[a]

(cal_{th} = 4.184 J)

	1	2	3	4	5	6	7
m'(compound)/g	0.672225	0.688259	0.689959	0.691483	0.706798	0.713814	0.720016
m''(auxiliary oil)/g	0.079163	0.068885	0.067380	0.066104	0.051789	0.043876	0.038964
m'''(fuse)/g	0.001098	0.001106	0.001017	0.001001	0.000833	0.001030	0.001056
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
Δt_c/K = $(t_f - t_i + \Delta t_{corr})$/K	1.984647	1.998490	2.001331	1.999425	1.999988	1.997161	2.000148
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-7949.54	-8004.99	-8016.37	-8008.73	-8010.99	-7999.66	-8011.63
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-9.99	-10.00	-10.01	-9.99	-9.98	-9.99	-8.80
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	0.00	9.51	0.00	0.00	0.00	0.00
$\Delta E_{(corr\ to\ std\ states)}/cal_{th}$[c]	3.24	3.28	3.22	3.28	3.30	3.30	3.31
$\{-m''(\Delta E_c^\circ/m)(auxiliary\ oil)\}/cal_{th}$	871.14	758.04	741.48	727.44	569.91	482.83	428.78
$\{-m'''(\Delta E_c^\circ/m)(fuse)\}/cal_{th}$	4.45	4.48	4.12	4.05	3.37	4.17	4.28
$\{m'(\Delta E_c^\circ/M)(RJ\text{-}6)\}/cal_{th}$	-7080.52	-7249.01	-7267.87	-7283.77	-7444.21	-7519.17	-7583.88
$\{(\Delta E_c^\circ/m)(RJ\text{-}6)\}/cal_{th}\ g^{-1}$	-10532.97	-10532.40	-10533.77	-10533.56	-10532.29	-10533.79	-10532.95
$\{(\Delta E_c^\circ/m)(RJ\text{-}6)\}/cal_{th}\ g^{-1}$	-10533.10 ± 0.24 (mean and standard deviation of the mean)						

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ϵ^i(cont)$(t_i - 298.15\ K) + \epsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Item 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

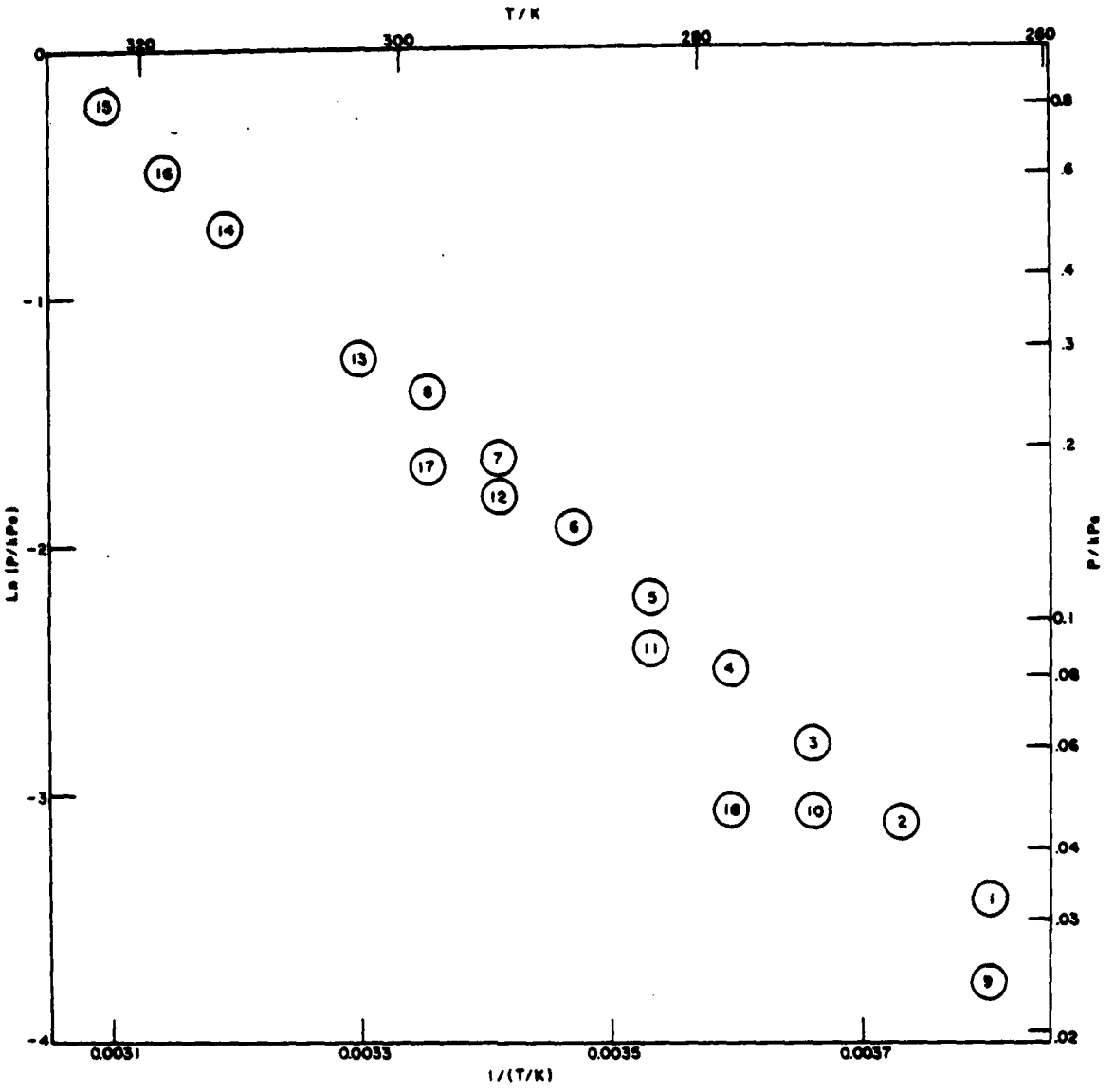


FIGURE 1. Measured values of vapor pressure of JP-10 at various temperatures, plotted as ln P versus 1/T. The sequence in which the data points were obtained is shown by the numbering of the points.

Kinetics of Hydrocarbon Oxidation/Grant AFOSR 77-3215

R. R. Baldwin and R. W. Walker

Department of Chemistry, Hull University
Hull, England.

For a number of years, the research group at Hull has been concerned with elucidating the mechanism of oxidation of hydrogen, carbon monoxide, alkanes, alkenes, aldehydes and related compounds and in evaluating the rate constants and Arrhenius parameters of the elementary free radical reactions involved. Such information is essential for the modelling of atmospheric pollution problems, of the combustion processes in the internal combustion engine and in gas turbines and rocket engines. The experimental work at Hull is conducted mainly in the temperature range 400-600°C, and so forms a convenient link between room temperature studies using flash photolysis, flow discharge and other techniques, and high temperature studies using shock tubes or flames.

Three main methods of approach have been used.

1. The addition of traces (0.01-1%) of reactant (alkane, alkene, etc.) to slowly reacting mixtures of $H_2 + O_2 + N_2$. Such studies provide information in two areas.

(a) Rate constants for the reaction of H atoms and OH radicals with the additive.

(b) The subsequent reactions of the radicals produced from the additive. As detailed in published papers, this approach has a number of advantages over direct studies of the oxidation of the alkane or alkene.

2. The oxidation of aldehydes in the temperature range 450-540°C. Although aldehyde oxidation is a complex process at temperatures below 400°C, the mechanism becomes much simpler at higher temperatures and hence may be used as a controlled source of radicals. Moreover, in contrast to the position with alkane oxidation, the products are much less reactive than the parent aldehyde, so that the complications of alkane oxidation are largely avoided.

3. The decomposition of tetramethylbutane (TMB) in the presence of O_2 has recently been found to be a convenient source of both t-butyl radicals and HO_2 radicals, enabling the reactions of these radicals to be studied.

Experience has shown that progress is best achieved with certainty by a multi-channelled approach in which all methods of

attack are used. As a result, considerable progress has been made over the last two years in a number of areas indicated below.

1. The mechanism of alkane oxidation

As reported at a previous Contractors' Meeting, the main types of reaction involved in the initial stages of alkane oxidation in the temperature range 400-600°C have been identified, rate constants have been obtained for most of the elementary steps in the oxidation of C_2-C_5 alkanes, and patterns in the rate constants and Arrhenius parameters of the reactions involved have been recognised. As a consequence, the initial stages in the oxidation of an alkane not previously studied can now be predicted with reasonable accuracy by the use of rate constants obtained from the study of lower alkanes. This is an important development, since it is obviously impossible to evaluate experimentally the rate constants for all the elementary steps involved in the oxidation of all hydrocarbons.

2. The mechanism of alkene oxidation

In the temperature range 400-600°C, conjugate and lower alkenes are major products in the initial stages of alkane oxidation. Consequently, for a full modelling of the oxidation process for alkanes, the mechanism of alkene oxidation must be understood. Very few studies of alkene oxidation have been made, and these studies have provided little information on the mechanism of reaction and on the rate constants of the elementary reactions involved. This is not altogether surprising since both H-abstraction from the alkene by radicals, and radical addition to the alkene, are possible. From the studies at Hull, either a detailed study in the case of some alkenes or observations incidental to a study of a related alkane, the main types of reaction involved are now becoming clear for the first time. Although H-abstraction from alkenes which usually leads to the formation of a resonance-stabilised alkenyl radical, has not been detected in low temperature studies, it has been found to play an important part in the temperature range 400-600°C. A number of rate constants have been evaluated, and patterns in these rate constants are becoming apparent.

3. Reactions of HO_2 radicals

Relatively few rate constants for HO_2 have been available until recently, partly because of the difficulty of finding clean and reproducible sources of HO_2. All three approaches indicated earlier have been used to obtain rate constants for the reaction of HO_2 radicals with H atoms, H_2, CO, with the aldehydic CH and side chain CH bond in a range of aldehydes (HCHO, C_2H_5CHO, $n\text{-}C_3H_7CHO$ and $i\text{-}C_3H_7CHO$), with the alkanes C_2H_6 and tetramethylbutane, and with alkenes such as C_2H_4 and $i\text{-}C_4H_8$.

4. Thermodynamic properties of alkyl radicals

Studies of the decomposition of 2,2,3,3-tetramethylbutane and of 2,2,3-trimethylbutane have enabled values of the enthalpy and entropy of both $t\text{-}C_4H_9$ and $i\text{-}C_3H_7$ radicals to be obtained. The results suggest that the bond dissociation energies of alkanes are significantly higher, by about 10 kJ mol^{-1}, than the presently accepted values. Recommended values are given below.

R	CH_3	C_2H_5	$i\text{-}C_3H_7$	$t\text{-}C_4H_9$
$D^{\circ}_{298}(R\text{-}H)$/kJ mol^{-1}	438.5±1.0	420.5±4.0	402.5±4.0	390.2±2.0

Future Work

In the immediate future, three main objectives are visualised.

1. To reinforce the present understanding of the processes involved in alkene oxidation by examining in more detail the oxidation of those alkenes (butene-1, butene-2, i-butene, pentene-1 and pentene-2) which have so far only been superficially studied.

2. To continue to exploit the decomposition of tetramethylbutane in the presence of O_2 as a source of HO_2 radicals so as to study the reaction of HO_2 radicals with alkanes, alkenes and related substances, as well as the ease of destruction of these radicals on various surfaces.

3. To examine possible sources of resonance-stabilised alkenyl radicals, such as the allyl radical ($CH_2CH{=}CH_2$) whose oxidation reactions have not been elucidated. Reactions of these radicals are particularly important at temperatures above 500°C.

Publications since the last Contractors' Meeting

1. "Rate constants for hydrogen + oxygen system, and for H atoms and OH radicals + alkanes", R. R. Baldwin and R. W. Walker, J. Chem. Soc., Faraday I, 1979, 75, 140.

2. "Carbon dioxide formation in oxidation of propionaldehyde", R. R. Baldwin, K. A. Lewis and R. W. Walker, Combustion and Flame, 1979, 34, 275.

3. "Oxidation of isobutyraldehyde in aged boric-acid-coated vessels", R. R. Baldwin, C. J. Cleugh, J. C. Plaistowe and R. W. Walker, J. Chem. Soc., Faraday I, 1979, 75, 1433.

4. "Addition of 2,2,3,3-tetramethylbutane to slowly reacting mixtures of hydrogen and oxygen", R. R. Baldwin, R. W. Walker and Robert W. Walker, J. Chem. Soc., Faraday I, 1979, 75, 1447.

5. "Reaction of t-butyl radicals with hydrogen and with oxygen", G. A. Evans and R. W. Walker, J. Chem. Soc., Faraday I, 1979, 75, 1458.

6. "Decomposition of 2,2,3-trimethylbutane in the presence of oxygen", R. R. Baldwin, R. W. Walker and Robert W. Walker, J. Chem. Soc., Faraday I, accepted for publication.

7. "The addition of n-pentane to slowly reacting mixtures of hydrogen + oxygen at 480°C", R. R. Baldwin, Mrs. J. P. Bennett and R. W. Walker, J. Chem. Soc., Faraday I, accepted for publication.

COMBUSTION KINETICS OF SELECTED AROMATIC HYDROCARBONS
AFOSR-77-3384

Richard A. Matula and Richard C. Farmer

College of Engineering
Louisiana State University
Baton Rouge, Louisiana 70803

To assure adequate internal supplies of economical gas-turbine jet-fuels, the possibility of using coal and oil-shale syncrudes must be evaluated. A crucial step in this evaluation is the determination of the smoking and heating problems caused by the higher aromatic content of these newer fuels. The purpose of this study was to provide an inexpensive, broad data base of the high-temperature pyrolysis, oxidation, and carbon-formation process of selected aromatic hydrocarbon combustion systems so that potential combustor design problems could be recognized as quickly as possible.

The approach employed in this study was to conduct integrated experimental and analytical studies of the high temperature decomposition, ignition, and soot forming characteristics of selected aromatic hydrocarbons. Since commercial fuels are blended mixtures, rather than pure compounds, and since accurate kinetics models cannot be efficiently developed for mixtures, pure compounds were studied initially. In order to understand the combustion of pure multi-atom compounds, it is useful to know how homologous compounds react.

Shock-tube experiments were used to determine ignition and soot formation delay times, stable product distributions at intermediate states of combustion, and the amounts and rates of soot formation. Pressure and laser attenuation measurements supplied the basic data from the experiments. The composition of quenched gas samples was determined by gas chromatography. Existing computer programs have been utilized to describe the thermodynamics and kinetics of the flows of interest. Extensive development of pertinent thermodynamic data of polycyclic hydrocarbons has been necessary before appropriate calculations could be made.

Conditions under which soot forms, the delay time that it takes to start forming soot, the amount of combustible mixture which becomes soot, and the apparent initial soot formation rate were all determined for toluene/argon and toluene/oxygen/argon mixtures. Other fuels, such as benzene, hydrogen and acetylene were also studied for comparison. Results of these studies showed that condensation and dehydrogenation are the predominant steps of soot formation from aromatics. The concentration of intact

ring structure present is directly related to the sooting ability of aromatics. Ring rupture apparently occurs at about 1800K; hence, maximum soot conversion occurs at this temperature. This behavior is a very weak function of pressure; however, increased pressure does increase sooting below 1800K. Oxygen is an excellent suppressing agent to prevent soot formation. The carbon to oxygen atom ratio in a mixture and the temperature of the mixture at 5 atm pressure determining whether or not the mixture forms soot. The behavior of toluene mixtures was studied in detail. Soot was observed to form for carbon to oxygen ratios as low as 0.85. At temperatures below 1400K, soot did not form because no reactions occurred. A high temperature limit for soot formation exists; this limit may be predicted if soot is assumed to behave like the polycyclic aromatic hydrocarbon $C_{96}H_{24}$. If soot is assumed to behave like graphite, the high temperature limit is over predicted. Rates of soot formation have been measured and correlated.

Previously, ignition delay times for toluene, benzene, cyclohexane, cyclopentane, iso-cotane, and n-heptane have been measured and compared using the same shock-tube equipment. Such comparisons are useful because of the large disparity which frequently exists in experimental ignition data. A detailed study of toluene oxidation was also accomplished for two reasons. The basic data was desirable, and a determination of the precision with which such measurements can be made needs to be established. Our data identity the importance of shock-attenuation by the tube boundary layer and shock-acceleration in the reflected shock region as being critical in controlling measured ignition delays. Furthermore, these effects have been quantitatively evaluated. These questions are increasingly important as larger gas molecules (such as those comprising aromatic fuels) are studied.

All ignition delays, soot formation rates, and soot formation delays in the toluene mixtures have been correlated with an equation of the form:

$$\tau = A \exp\{+E/RT\}[\text{fuel}]^a[\text{oxygen}]^b[\text{argon}]^c$$

where τ is the delay or rate being correlated,
A is an apparent collision frequency,
E is an apparent activation energy,
R is the universal gas constant,
T is temperature,
a,b,c are power dependencies of the fuel, oxidizer, and diluent, respectively.
[] denotes concentration.
Specific values of the correlation parameters determined by our experiments appear in our final report on this project.

FUNDAMENTAL CHARACTERIZATION OF ALTERNATIVE FUELS EFFECTS IN CONTINUOUS COMBUSTION SYSTEMS

(Prime DOE Contract No. DE-AC03-77-ET-11313)

E. Wong
P. T. Harsha
R. B. Edelman

Science Applications, Inc.
21133 Victory Boulevard, Suite 216
Canoga Park, California 91303

The advent of alternative fuels has prompted investigations directed toward developing an understanding of their effects in practical combustion systems. Syncrudes obtained from coal, oil shale and tar sands typically have a higher aromatic content, a lower hydrogen-to-carbon ratio and are more viscous and less volatile than petroleum based liquids. This program involves an on-going interrelated theoretical and experimental effort with the overall objective being to provide data bases and engineering models designed to aid in the effective utilization of these fuels in continuous combustion systems. Chemical and aerodynamic processes are being investigated in order to develop the elements necessary to implement a validated coupled model of continuous flow combustors.

The results to be presented here will cover the chemical aspects of the problem with emphasis on soot formation. Quasiglobal kinetics modeling is being extended to include a series of additional subglobal steps found to be necessary to characterize the net soot emissions data being generated at Exxon Engineering and Research Co. under the direction of Dr. William Blazowski. A jet stirred combustor is currently in use and represents a laboratory analogue of primary zones with intense backmixing which are encountered in many practical combustion systems. The iterative procedure employed in developing the model utilizing the data from this laboratory combustor, along with comparisons of predictions with data, will be discussed. Future work will also be outlined.

AFOSR, AEROSPACE SCIENCES, CONTRACT NO. F49620-77-C-0111

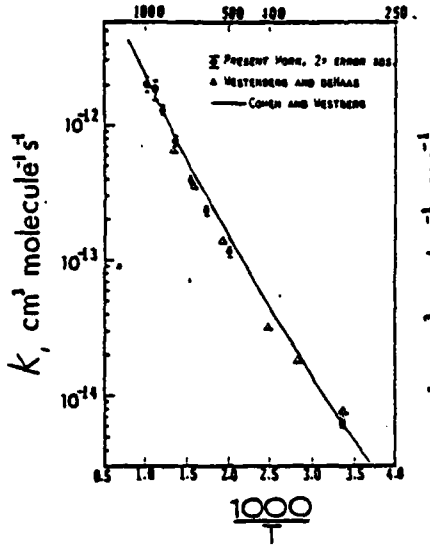
F. P. Tully and A. R. Ravishankara

Molecular Sciences Group
Engineering Experiment Station
Georgia Institute of Technology
Atlanta, GA 30332

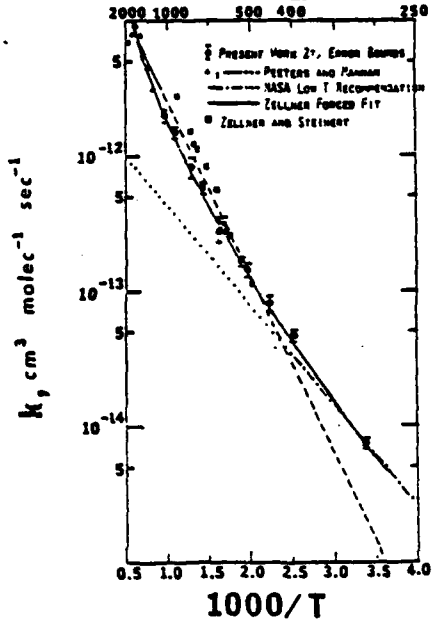
Under AFOSR Contract No. F49620-77-C-0111 we are measuring absolute rate constants for elementary bimolecular free radical reactions of importance to the generation of a predictive understanding of hydrocarbon combustion processes and advanced fuel reactivity in aircraft and rocket exhaust plume environments. These measurements significantly contribute to the chemical kinetics data base used by aerospace engineers as input to solutions of problems involving air-breathing engines and advanced component rocket plumes. The experimental technique used in this program is (laser/spark discharge) flash photolysis -- (resonance/laser induced) fluorescence. Direct measurements of absolute rate constants for selected radical oxidant-molecule reactions are made in the temperature interval 300-1200K at pressures between 20 and 800 Torr. Specific reactions from among the sequence OH + H_2, D_2, CH_4, C_2H_6, C_3H_8, CH_2O, HCl and OH,OD + CO and O + HCl are being investigated. Correlations between the measured experimental data and the predictions of theoretical models are being examined.

During the past year we have completed studies of the reactions OH + H_2, CH_4, CO, and C_2H_6 → Products. Direct rate constant measurements have been made in the heretofore only marginally accessible temperature range up to above 1000K. As can be seen from the figures below, significant Arrhenius graph curvature has been observed for each reaction. Details of these studies will be discussed.

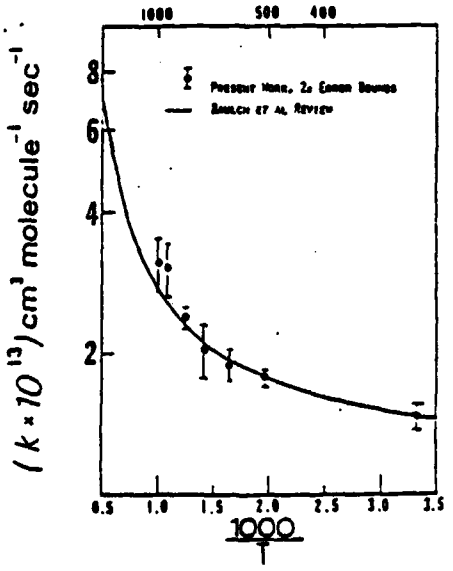
$OH + H_2 \rightarrow H_2O + H$



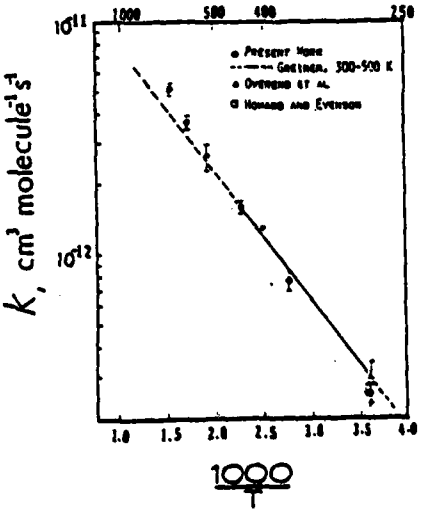
$OH + CH_4 \rightarrow H_2O + CH_3$



$OH + CO \rightarrow CO_2 + H$



$OH + C_2H_6 \rightarrow H_2O + C_2H_5$



FUEL COMBUSTION RESEARCH/CONTRACT F49620-78-C-0004

I. Glassman and F.L. Dryer

Department of Mechanical and Aerospace Engineering
Princeton University
Princeton, New Jersey 08544

Recognizing the uncertainties as to future available fuel sources and characteristics, the problems that could arise in military power plants from the use of coal derived liquids, petroleum derivatives from oil shale, secondary and tertiary recovery, etc., and the necessity for combustor modelling to facilitate rapid development of power plants using such fuels, AFOSR established at Princeton a "Center of Excellence" in Combustion-Related Fuel Problems. The program concentrates on chemically related combustion problems and has seen a cooperative effort between members of the Department of Mechanical and Aerospace Engineering and the Department of Chemistry.

Current research efforts encompass the pyrolysis and fuel rich oxidation of aliphatic hydrocarbons, the pyrolysis and oxidation of aromatic compounds, soot formation and destruction processes, and the methodology/application of sensitivity analysis techniques to combustion problems. As evidenced in our publications, understanding in each of these areas has contributed to further progress in the others to give a true integrated program. Attention is focused on problem areas associated with both current and future fuel properties.

Our studies of propane pyrolysis have been completed and submitted for publication.[1] The overall pyrolysis has been described by a first order rate expression with E_A = 58.65 kcal/mole and A = 3.2×10^{12} s^{-1}. The expression agrees well with previously reported rate data. In addition, a kinetic mechanism involving 13 chemical species and 31 elementary reactions has been postulated to describe the kinetics. Primarily the detailed experimental reaction composition data from our flow reactor were used to verify the mechanism, and comparisons with results from static vessel and shock tube experiments reported in the literature showed the extent of the validity of the proposed mechanism. Very good agreement over the temperature range 800 K to 1400 K and over the pressure range of 0.1 to 8.5 atm was obtained by adjusting 3 rate constants. The reactions in question are

$$CH_3 + C_3H_8 \rightarrow CH_4 + iC_3H_7 \quad (1a)$$

$$CH_3 + C_3H_8 \rightarrow CH_4 + nC_3H_7 \quad (1b)$$

$$H + C_2H_4 \rightarrow C_2H_3 + H_2 \quad (2)$$

We thus argue that the sum of the rate constants for Reactions 1a and 1b and the rate constant for Reactions 2 are best represented by

the expressions

$$k_{1a} + k_{1b} = 10^{15.35} \exp(-25140/RT) \text{cc/mole-s}$$

$$k_2 = 10^{12.77} \exp(-5000/RT) \text{cc/mole-s}$$

These propane pyrolysis results have been extremely useful in our study to develop global kinetic oxidation expressions for propane and the alkanes in general.

The long range efforts in our study of pyrolysis and oxidation of aromatics are directed at understanding the detailed reaction kinetics. However, one of our early objectives is determine whether under combustion-like conditions some carbon dioxide forms from a mechanism other than carbon monoxide oxidation as we detailed in recent reviews [2,3]. If so, the implications with respect to soot formation from aromatics in pre-mixed flames are very great.[4] The early experiments with toluene in the flow reactor revealed difficulty in making a carbon balance and sampling handling and analysis. Consequently our major experimental effort of the past year in this area has been to developing an improved heated sampling and storage approach and analysis procedures. We have noted that single-sample-analysis of permanent gases, light hydrocarbons, and higher hydrocarbon intermediates results in substantial limitations of the packed columns which can be used and/or in very long analysis times. Capillary column techniques are ideal for heavier hydrocarbon separation, but they cannot be employed simultaneously with packed columns and do not separate light hydrocarbon and permenent gases. Thus the sampling system we have developed has as an integral part the addition of systems which permit

i) continuous analysis of oxygen (by paramagnetic detection) and of hydrogen (by catalytic conversion to and detection of water vapor).

ii) simultaneous acquisition at each sampling position of two heated gas samples which will thus permit simultaneous operation of the HP5985GS/MS system for heavy hydrocarbon analysis, and the HP5840GC for CO, CO_2 and light hydrocarbon analysis.

The simultaneous acquisition approach has been designed such that if it is warranted, simple modifications can be made to include continuous analysis for CO/CO_2 by non-dispersive infrared techniques. A hot-water cooled (90C) sampling probe system has been completed and prototype heating sampling valve system permitting simultaneous storage of up to sixteen samples, in each valve, has been fully evaluated and is now operational. Thus flow reactor studies have again begun.

Not only have extensive experimental results been obtained [5] in that aspect of our program concerned with soot formation and destruction processes, but after extensive review of the literature

phenomenological models of soot processes in combustion systems have been put forth.[4] These models are based on relatively new concepts as to the important precursors to soot formation. The essential element is that it is the rate of formation of conjugated hydrocarbon species which have polar resonance structures which determine the tendency of a fuel to soot. In particular, butadiene and its carbonium ion are the most prominant candidates as precursors, rather than acetylene. Indeed butadiene and the C_4 olefins have been found to have a greatest propensity to soot.[5] Making use of our kinetic studies, it has been concluded that in pre-mixed flames the dominant factor which controls the tendency to soot is the flame temperature. Further, the aromatics appear to soot more readily due to their mode of oxidation through formation of carboxyl groups. Thus aromatics at a given stoichiometry are "more fuel rich" than the aliphatics.[4]

For diffusion flames it has been concluded that temperature and fuel structure are the dominant factors which determine the tendency of a fuel to soot. The temperature controls the rate of the fuel pyrolysis, and the structure the ease with which the important precursors form.

The support for these conclusions have been based upon carefully planned fuel jet experiments with judicious choice of additives. According to their ability to reduce or increase the sooting tendency of a diffusion flame, it was found that additives could be distinguished into two classes. Most diluents were found to act as if they were inert gases in decreasing a fuel tendency to soot. The effectiveness of such diluents was found to be proportional to their molar specific heats. Thus, it was demonstrated that not only was the effect of N_2 and Ar thermal, but so were the effects of CO_2, SO_2 and water vapor. Non-inert additives such as N_2O, O_2 and Freon 12 increase the sooting tendency substantially when trace amounts are added to the fuel jet. Halogenated compounds appear even more effective than oxygen containing species. The indications are that the oxidizer dissociate in the fuel close to the flame front. Halogen or oxygen atoms so formed attack the abundant fuel and dehydrogenate it rather than remove H atoms from the system. This result further supports one of our major contentions that the initial pyrolysis of the fuel is the crucial step in soot formation in diffusion flames.

Other very significant diffusion flame experiments have recently been completed. By measuring the sooting height of various fuels as a function of their flame temperature, which was controlled by N_2 dilution, it has been shown that at a given temperature the C_4 olefins have the greatest propensity to soot - far greater than even acetylene. Others have shown that butadiene soots more readily than the aromatics.[6]

In addition to the above studies research is also underway under the direction of Prof. H. Rabitz of the Department of Chemisty on

applications of sensitivity analysis to complex combustion problems. Sensitivity analysis allows for the probing of which kinetic or transport parameters significantly contribute to particular combustion observables. In its simplest form the technique yields partial derivatives of chemical species concentrations with respect to system parameters such as initial concentrations or rate constants. This information is a valuable guide to the underlying kinetics and could also be used for the planning of new experiments. The use of sensitivity gradients is particularly helpful for complex combustion systems with many possible kinetic pathways. An algorithm for performing the necessary calculations has been prepared and calculations are in progress for the analysis of flow reactor combustion systems.

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FREE RADICALS OF IMPORTANCE IN AIR-BREATHING COMBUSTION REACTIONS

D. M. Golden
SRI International, Menlo Park, CA 94025

Understanding of the complex problem of combustion requires a model which can be used to predict various observables of interest [i.e., flame speed, energy release, time-dependent concentrations profiles, temperature (assuming thermal equilibrium)] for a wide range of initial conditions (temperature, pressure and composition). Even if such a model were only able to provide qualitative guidelines, it would be useful in consideration of design parameters for various combustors as well as for a foundation for the modification of various fuels.

The research that is reported on here is motivated by the need to supply a well understood chemical kinetic data base for the model alluded to above. There are so many elementary chemical processes involved that it is essential to develop methods for estimating the least sensitive of these while concentrating on the experimental determination of the most sensitive.

Among the most important types of data necessary are heats of formation of relevant free radicals. Some recent experiments which address the question of the heats of formation of various radicals will be discussed.

In addition, the development of new techniques employing infrared lasers as radical generators will be discussed. Experiments that enable the determination of radical-molecule reaction rate constants over a large temperature range will be described.

The use of isothermal laser pyrolysis as a method for determining homogeneous rate constants and products for surface-sensitive materials will be described. Planned use of laser-induced flourescence techniques in conjunction with this method will also be described.

RESEARCH NEEDS IN TURBOPROPULSION COMBUSTION TECHNOLOGY

Dr. James S. Petty

Aero Propulsion Laboratory
Air Force Wright Aeronautical Laboratories

In 1978 a joint Air Force-Navy-Army team conducted a broad survey of the U.S. aircraft turbine engine manufacturers to assess the status of turbopropulsion combustion technology. The conclusions of this assessment team are being published as an Air Force Aero Propulsion Laboratory technical report (AFAPL-TR-79-2115). One result of this assessment has been the preparation of a new AFAPL five-year combustion technology plan.

This presentation will review the combustion technology assessment and the technology plan, with primary emphasis on those areas in which basic research needs exist. These needs involve fluid and solid mechanics, heat transfer, combustion and numerical analysis in the area of main burners, afterburners, combustion modeling, structural and mechanical design and alternative fuels.

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THURSDAY

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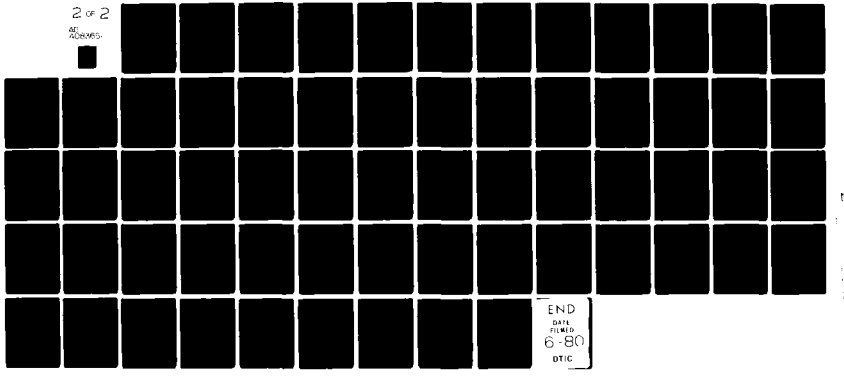

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Fundamental Modeling of 3-Dimensional 2-Phase Reacting Flow Systems

(AFOSR-74-2682)

J. Swithenbank, A. Turan, J. Dutt

In previous USAF sponsored work, (AFOSR-74-2682), combustor modeling techniques based on both finite difference algorithms and stirred reactor network models have been investigated. These were novel in that they incorporated spray evaporation and chemical kinetic aspects and were intended to aid the design of practical gas turbine and ramjet combustors.

In the first stage of the present program, these techniques have been tested critically by running the computer model and the experimental rig at the identical air mass flow, fuel flow (AFR=30), inlet temperature, pressure and droplet size distribution at both hot and cold conditions. The results showed that the model correctly predicted all aspects of the flow within experimental accuracy. One interesting observation concerned the exit velocity distribution. In the cold flow case, both theory and experiments showed a large peak at the center. In the hot flow case, the peak in velocity disappeared in both the predictions and the experiment although it was still present in the mass flow distribution. This anomaly was due to the fact that a low temperature region existed close to the axis when combustion was present. If this phenomenon is a general feature of hot flow, it could be used to speed up the computations and thus help solve one of the biggest problems in 3-dimensional modeling procedures. Mathematical modeling techniques are currently being applied to ramjet dump combustors and steady process can be reported at this stage.

An interesting new experimental technique has been developed for studying the characteristic stirred and plug flow reactor networks. This is based on the application of pseudo-random tracer pulses to a water model of a test combustor. The responses at various points within the combustor are detected and the results are extracted by appropriate transformations and correlations applied to the discrete data samples. This generalized least squares algorithm yields the various transfer functions in terms of the impulse response and micro-mixing 'noise'. The experimental impulse responses can be interpreted in terms of the network interconnections, flows and volumes whilst the 'noise' information can be used to determine the mixedness of individual reactors in the network. It is hoped that this novel technique can be applied to hot combustors, possibly using a mercury vapour tracer, in future studies.

DETAILED MODELLING OF COMBUSTION PROCESSES

Elaine S. Oran and Jay P. Boris

Laboratory for Computational Physics
Naval Research Laboratory
Washington, D. C. 20375

This presentation summarizes the current research at NRL in the development and application of detailed modelling to combustion systems. Here detailed modelling is defined as the use of advanced numerical techniques to solve the time-dependent conservation equations for mass, momentum and energy on the time and space scales of interest. In combustion, this is often a multi-dimensional, multi-fluid, multi-phase problem with complicated boundary conditions. The simultaneous use of empirical and phenomenological submodels is required to describe processes whose scales cannot be resolved in the calculation or whose evaluation would require independent ab initio calculations.

The current work at NRL falls into five main research areas:

I. Development of numerical techniques,
II. Ignition and extinction of flames,
III. Turbulence phenomena,
IV. Supersonic reactive flows, and
V. Chemical kinetics and thermophysical properties of materials.

These include work in complicated fluid flows with simplified chemistries, simple flows with extensive, detailed chemistries, research to determine best or adequate chemical kinetics reaction rate schemes, and simulations of large-scale combustion systems. The focus has been on intrinsically time-dependent phenomena and the study of the interplay of the fluid dynamics and the energy released from chemical reactions. Recent progress and the ongoing work in each of the five areas listed above will be summarized and reviewed.

The first and most extensive part of the work at NRL has involved developing and extending a number of algorithms and then developing asymptotic timestep splitting techniques for coupling the physical processes they represent. The Flux-Corrected Transport (FCT)[1] algorithms have been incorporated in multi-dimensional flame and detonation models.[2,3] A Lagrangian algorithm, ADINC,[4] has been developed to study systems where the characteristic velocities are subsonic. Triangular gridding techniques[5] have been developed for the study of incompressible flows with complicated boundaries and free surfaces. This method is now being extended to compressible and three-dimensional flows.

The research in flame ignition and extinction has involved developing simplified models for predicting whether a gas mixture will ignite[6] and in using detailed flame models to determine the flammability limits of materials.[7] Current work is focused on studying the effects of diluents as a flame suppressant, which is the basic idea of the N_2 pressurization method for putting out fires in enclosed chambers. Work is also in progress to develop a model for the quench volume of a flammable gas mixture which includes the effects of buoyancy and molecular diffusion. This model will be benchmarked against the results of detailed one- and two-dimensional simulations.

The collaboration with the University of Sheffield is a natural extension of the laminar flame studies mentioned above and the more fundamental turbulence studies summarized below. The two-dimensional flame model[2] is currently being modified to simulate a gas jet with material entering at the bottom of the mesh and leaving at the top. The object of this study is to make detailed comparisons with the experimental work at Sheffield.[8] Studies will be made of both cold jets and flames to evaluate quantitatively the underlying mechanisms of the macroscopic features and instabilities observed.

Research in the basic mechanisms of turbulence has involved detailed studies of fundamental fluid instabilities.[9,10] The goal is to understand the mechanisms and then to parameterize the results in a phenomenological model that can be used in large detailed simulations. Such a model will be essential when we look at the turbulence regime in the Sheffield flame.

The FCT algorithms mentioned above are particularly useful to study shocks and detonations. They have been used to study detonation phenomena in one-dimension[3] and they are the bases of a two-dimensional model which is being used to study the cellular structure of propagating detonations. This work has necessitated the development of an induction parameter model to represent the amount of energy released and product formed on very short timescales. The model is being calibrated against a full simulation which incorporates a complete chemical kinetics scheme.

Finally, a research effort has been initiated in collaboration with the Chemistry Division at NRL, and Science Applications, Inc., to develop and test chemical reaction rate schemes for use in detailed models. Our previous efforts have involved developing and testing schemes for H_2-O_2[11] and CH_4-O_2.[12] The current work is a study of the oxidation of aromatics, starting with benzene. This will involve experimental work using instruments such as the shock tube and fast flow reactor in combination with theoretical calculations and numerical simulations.

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Overview of DOD Colloquium on Gas Turbine Combustor Modeling

S.N.B. Murthy
Purdue University

Abstract not received

OVERVIEW OF MRC COLLOQUIUM ON DYNAMICS AND MODELING OF REACTIVE SYSTEMS

J. Ray Bowen

Department of Chemical Engineering
and
Mathematics Research Center[+]
University of Wisconsin - Madison

The MRC's primary objective has been to engage in unclassified, basic research in applied and applicable mathematics. Areas which are considered to be relevant or potentially applicable to Army problems are applied analysis, physical mathematics, numerical analysis, statistics, probability, operations research, and computer sciences. Physical Mathematics refers the area of applied mathematics with following characteristics:

> "(a) The primary motivation comes from physical problems in continuum mechanics.... .
>
> (b) Mathematics is regarded as a tool rather than an end in itself. The objective is to solve specific equations using not only the most efficient available method but also developing new techniques when existing methods are inadequate."[*]

As part of the effort in physical mathematics, the MRC held the Advanced Seminar on Dynamics and Modeling of Reactive Systems[+] on October 22-24, 1979. This paper is an overview of the seminar. The unifying theme of the fifteen papers was the mathematical modeling of physical problems in which one must account for interaction between some reaction mechanism[&] and convective-diffusive transport of matter and energy. Although in general the reaction mechanism is the source of nonlinearity, there are some physical problems in which significant nonlinear effects may arise from the diffusive terms. The approach to these problems varies somewhat with the application.

In chemical reactor engineering one is concerned because some reactive-diffusive systems are not well behaved, that is the system does not always proceed monotonically in time (or space) to a unique state of completed reaction. Instead some systems exhibit temporal (or spatial) oscillations, which rather than decaying, become temporally (spatially) periodic with a finite amplitude. In other instances the amplitude of the oscillations becomes very large, while in others the oscillations are chaotic rather than periodic. Some instances also are

capable of multiple steady states. As a consequence several contributions by chemical engineers, were concerned with questions of multiplicity of steady states, stability of a steady state, sensitivity of the steady state to small changes in the physical parameters and oscillatory behavior of solutions.

The contributions specifically concerned with combustion were a general review of the current challenges in combustion research, an analysis of nonisobasic flame propagation, and a discussion of closure and character of the conservation equations for heterogeneous two phase flow. The analysis of aerosol dynamics and periodic precipitation phenomena were the subjects of two contributions, while one paper was a survey of the techniques for measuring or estimating chemical kinetic parameters.

The advanced seminar not only served as a forum for the discussion of new results but also provided an opportunity for identification of new challenging problems in the solution of mathematical models.

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* Quotes from Preliminary Draft of Proposal for MRC contract 1979-85 July 14, 1978.

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Here reaction mechanism has a broad definition to include physical processes such as droplet coalescence and precipitation as well as chemical transformations.

RADIATION AUGMENTED COMBUSTION

Contract No. F49620-77-C-0085

M. Lavid, A. E. Cerkanowicz, W. S. Blazowski

Exxon Research and Engineering Company
Corporate Research-Technology Feasibility Center
Linden, New Jersey 07036

Present aircraft operational limitations which are encountered due to combustion associated phenomena such as flammability, flame propagation, ignition and stable combustion may be alleviated by employing a number of advanced practical techniques. One of these techniques is radiation augmented combustion utilizing selected wavelengths of vacuum ultraviolet (VUV) and of ultraviolet (UV) radiation.

The ignition and combustion enhancement of typical gaseous and liquid fuel-air mixtures used in air-breathing propulsion engines by vacuum ultraviolet or ultraviolet radiation is achieved by selectively producing reactive intermediates via a photodissociative mechanism or combined photo-thermal methods.

The intermediate of major importance in the initiation of practical combustion reaction using VUV radiation is atomic oxygen, which can be efficiently produced by photodissociation of oxygen with radiant energy below 180 nm.

Invoking a phase plane analysis, it can be shown that ignition can be achieved via two paths; namely, thermal and photochemical. The former involves a temperature rise such that the thermodynamic state of the mixture moves into the rapid reaction region. The latter need not involve a temperature rise; instead an increase in concentration of a reactive intermediate (oxygen atom) is achieved which moves the thermodynamic state of the mixture to the rapid reaction region via photodissociation. The photochemical (radiative) path results in completely different ignition characteristics than the conventional thermal path.

In addition to the formation of a photochemical ignition kernel, the radiative technique also provides for the creation of regions of photochemical combustion enhancement, by favorably altering the reaction kinetics. The radiative enhancement is achieved by either photochemically increasing the concentration of reactive radicals, resulting in reduced reaction time in the combustion region and consequently the realization of enhanced flame propagation; or by photodissociation of a degenerate combustion intermediary species, thereby removing any degenerate chain branching steps in the combustion kinetics.

Experimental results obtained in Exxon Corporate Research Laboratories have extended our detailed understanding of the radiative ignition technique and have established a reasonable proof of the combustion enhancement concept. All the experiments were carried out in a horizontal cylindrical combustion chamber under stationary conditions with various premixed combustibles. For the radiative ignition experiments two different light sources have been used: pulsed and continuous. It was found that the pulsed light source successfully ignited different combustible mixtures with stored ignition energy of the same order of magnitude or less than that required for spark ignition. Furthermore, it was demonstrated for the first time that a suitable continuous light source is capable of igniting a combustible mixture. This paramount recent result implies the possibility of using an optical (imaginary) flame holder with zero pressure drop to stabilize combustion in primary combustors as well as afterburners.

The radiative enhancement experiments employed only continuous light sources. Preliminary results have shown up to 20% enhancement in flame propagation only in marginal flames, in particular, at very fuel lean ratios. These preliminary results demonstrate a potential opportunity to extend the combustor operating limits utilizing the radiative technique. It is construed that the enhanced flame propagation can be translated into higher combustion rate and extended stability limits.

During the course of the experimental work we have also developed the technical knowledge for designing an advanced optical/radiative light source. Furthermore, a comprehensive analytical model of radiative initiation and enhancement has been also developed to assist us in optimizing our experimental work.

The experimental results reported here give us confidence that radiative augmented combustion is a potential viable technique to extend current aircraft operating limits.

AIR FORCE SUPPORTED RESEARCH PROGRAM AND NEEDS ASSOCIATED WITH GAS TURBINE ENGINE EMISSIONS AND OTHER COMBUSTION RELATED PROBLEMS

Capt Harvey J. Clewell
Capt Joseph A. Martone

Environics Division (RDV)
Engineering and Services Laboratory* (ESL)
Air Force Engineering and Services Center (AFESC)
Tyndall AFB, FL 32403

The Environics Division (RDV) within the Air Force Engineering and Services Center's (AFESC) Engineering and Services Laboratory (ESL) is the Air Force laboratory focal point for environmental quality (EQ) research and development. In this capacity AFESC/RDV tracks the EQ related R&D efforts of all Air Force laboratories in addition to maintaining its own comprehensive multimedia (i.e., air, water, and solid waste) program which includes R&D efforts in environmental modeling, chemistry, planning and monitoring as well as in resource conservation, control technology and energy research. Most research and development is accomplished through industrial and university contracts many of which are jointly funded by organizations such as AFOSR, AFAPL, EPA, NASA and the Navy. Although the major AFESC/RDV research thrust is in exploratory development (6.2) and advanced development (6.3), a limited amount of Laboratory Director's funds are available for basic research (6.1).

Since aircraft gas turbine engines burning military aviation fuels are a pollution source of special Air Force interest, AFESC/RDV conducts R&D activities aimed to assure a fleet which meets Air Force aircraft engine emission goals and Federal, state, or local pollution regulations which affect military aircraft. Listed below are short descriptions of ongoing research projects that most directly relate to aircraft engine emissions and combustion dynamics and kinetics. Also included are descriptions of the combustion related efforts conducted in our energy R&D program. The list is an update of material presented at the 1978 AFOSR contractors meeting on air-breathing combustion dynamics.

*Formerly known as the Civil and Environmental Engineering Development Office (CEEDO)

a. Catalytic Combustor Development. The objective of this joint AFESC/NASA Lewis program is to demonstrate aircraft turbine engine main burner designs which employ catalytic combustion technology to achieve extremely low NO_x emissions at subsonic cruise. Phase I, which has been completed, consisted of the generation and analytical evaluation of several catalytic combustor concepts and preliminary design of the most promising concepts. Phase I results are summarized in NASA TM 79049 and final reports will soon be available (ESL-TR-79-23 and CEEDO-TR-79-03). General Electric was recently contracted to perform the 16 month Phase II effort which will consist of a series of tests, modifications, and retests to refine the most promising catalytic combustor configuration.

b. Variable Geometry Combustor Development. The variable geometry or air staging concept employs movable parts for regulating and varying the rate of airflow into varicus sections of the combustor. In effect the combustion zone equivalence ratio and local mass loading can be regulated. This fundamental characteristic has the potential to improve altitude relight, ground idle and starting problems and result in very low pollutant emissions. This concept is being examined for application to military aircraft engine combustors in a joint NAPC/AFAPL/AFESC contractual effort with Pratt and Whitney and Garrett Airesearch. Last year's work involved an in-depth review and analysis of variable geometry concepts with the selection of the most promising concepts for bench and/or sector testing in FY80. Phase II of the program (FY81-82) will involve a full scale performance/emissions evaluation and limited testing with a variety of fuels.

c. Fuel Character Effects Combustion Studies. It is inevitable that some changes in aircraft fuel specifications will be needed in the future in order to utilize alternate sources of crude stock and increase yields. However, before fuel specifications are relaxed, the impact on engine combustor performance, pollutant emissions and combustor life must be known. To meet this Air Force need, the AFAPL and AFESC began contractual fuel character effects studies in FY77. In these parametric studies, up to thirteen fuel blends with varying hydrogen content, aromatic structure, volatility and distillation end point are burned in a variety of combustor types. Studies on the J79, F101, and TF41 combustion systems are complete and final reports will soon be available (CEEDO-TR-79-06, CEEDO-TR-79-07, and ESL-TR-79-29 respectively). The emissions results for the J79 and F101 work are summarized in paper No. 79-37.3 presented at the 72nd annual meeting of the Air Pollution Control Association. In FY80, parametric fuel studies on the low smoke J79 combustor will be conducted at General Electric and a 3 year alternative fuels combustion research program jointly funded by AFAPL/AFESC and the Canadian Department of National Defense will be initiated. The latter effort will culminate with selected fuels tested in a PT6

and a JT15D combustor. The work may involve correlation of fuel properties with exhaust PNA levels. The emissions data from these combustion studies is being incorporated into our airbase air quality assessment model in order to facilitate the environmental impact analysis of future aviation fuels.

d. Microemulsions for Smoke Suppression. The Air Force has a continuing interest in controlling smoke emitted from jet engine test cells. The US Army Fuels and Lubricants Research Laboratory (ARLRL) located at Southwest Research Institute has had success with low smoke, fire safe diesel fuel microemulsions. In an effort to explore the smoke reduction potential of aviation fuel microemulsions, SwRI has been contracted to conduct fuel formulation and testing on a T-63 combustor. Preliminary work has shown that water, ethanol, and methanol in JP-4 and JP-8 microemulsions can significantly reduce baseline smoke levels. The results agree with earlier SwRI work that has shown the fuel hydrogen/carbon ratio as an important factor in controlling exhaust smoke. Work is continuing in FY80 to further evaluate fuel microemulsion sensitivities and investigate smoke suppressant fuel additive/microemulsion synergism.

e. Automatic Isokinetic Jet Engine Sampler. The Navy and AFESC have sponsored the development of an automatic isokinetic jet engine particle sampler. The sampler is undergoing evaluation at North Island Naval Air Station, San Diego. The fully automated sampler features a probe with a divergent supersonic inlet to allow isokinetic sampling up to Mach 1.4 and an electrical mobility aerosol analyzer for real time particle size analysis. In FY80 the sampler will be used to develop a correlation between SAE smoke number and true mass emissions. Up to 25 high and low smoke J79 engines burning both JP-4 and JP-5 will be used in the study.

f. USAF Aircraft Engine Emission Goals. The Air Force aircraft engine emission goals established in the early 70s are the basis for AFESC's involvement with low emission combustor development programs. Since then much has been learned about airport/airbase and stratospheric dispersion modeling of aircraft pollutants and about the limitations, development time, and costs of pollution reduction technology. In FY79 AFESC considered this new input in a reevaluation of Air Force emission goals. The final report (ESL-TR-79-30) will be available soon. The report concludes that carbon monoxide and oxides of sulfur are not serious problems at today's emission levels while smoke and hydrocarbon emissions appear to warrant the highest priority for reduction. Although cost effective oxides of nitrogen control is viewed with pessimism it is concluded that NO_x reduction deserves continued USAF research.

g. Fuel Additive Evaluation. Both the Navy and the Air Force have demonstrated that fuel additives such as ferrocene can reduce smoke from gas turbine engines. AFESC, AFLC, and NAPC

are sponsoring evaluations of ferrocene and another iron based additive, XRG using a variety of engines at Tinker AFB. Phase I of the study will involve the testing of 10 J57 engines. Tested engines will be returned to service and will be periodically inspected for any long term effects of additive use. Two J57 engines tested with ferrocene are presently accumulating flight hours. The engine types tentatively included in Phase II are the J75, TF30, TF33, and TF41.

h. Jet Engine Test Cell Particulate Control. The Air Force routinely tests turbine engines in fixed test cells, some of which have been cited by state pollution control officials for violations of opacity regulations. A theoretical study (CEEDO-TR-78-53) predicted that relatively low efficiency and low cost techniques could bring jet engine test cells into compliance with air pollution regulations. The system proposed included a water spray and a mist eliminator followed by a medium efficiency, high velocity, throw away type glass filter media. Unfortunately, a follow-on effort (ESL-TR-79-28) showed that rapid pressure drop build up across the filter would preclude practical application of glass filter media in test cells. A parallel study conducted at McClellan AFB (ESL-TR-79-19) showed that augmentor tube water spray normally used for cooling purposes also resulted in low efficiency removal (50 percent by weight) of engine smoke particles. In FY80 we will develop an analytical model to relate turbine engine test cell particulate emission characteristics to plume opacity and we will continue to consider low cost/efficiency test cell smoke control techniques.

i. Diffusion Battery Development. The size of smoke particles emitted from jet engine test cells is a critical parameter for predicting test cell plume opacity and for design of test cell pollution control equipment. Unfortunately, very few measurements are available, mostly because existing in-stack size classification instruments are not very reliable for the size range and mass loadings of interest. Accordingly the EPA and AFESC co-funded the design, fabrication and field testing of two prototype diffusion batteries capable of classifying particles between 0.025 and 0.2 micrometers diameter at stack temperatures up to 1000°F. Successful field tests were conducted at a test cell at Jacksonville Naval Air Station and evaluation of results, data interpretation and preparation of a draft final report are in progress.

j. Fuel Additive Mechanisms. A survey of possible mechanisms for the action of smoke suppressant fuel additives was recently carried out for AFESC by Professor Jack Howard of MIT. The final report (ESL-TR-79-32) provides a thorough review of both laboratory and full scale combustor tests of smoke suppressant fuel additives. Three different mechanisms are proposed for additives containing alkali metals, alkaline earth metals, and transition metals. In general, only metallic

additives appear to be effective, and there appears to be little promise for discovery of a novel additive concept. However, the present understanding of soot formation and burnout is extremely limited, particularly in complex acrodynamic flows, and more basic research is needed in this area.

k. Soot Formation and Burnout. To evaluate the impact of broadened fuel specifications on smoke emissions from gas turbine engines AFESC is sponsoring a study by Dr G. S. Samuelsen of the University of California, Irvine. This study is being carried out on a 3 inch diameter laboratory combustor designed to simulate the recirculating flow found in gas turbine combustion. Soot formation will be studied for a variety of simple gaseous and liquid fuels in both premixed and non-premixed modes. The effect of a smoke suppressant fuel additive will also be examined. Soot particle measurements will be made by probe extraction as well as by in-situ optical techniques. A major part of the effort, which involves personnel from Spectron Development Laboratory, will be devoted to development of optical techniques capable of providing particle concentrations and size distributions for particles as small as 20 nanometers in diameter. The soot will also be characterized by elemental analysis and Gas Chromatography/Mass Spectrometry. The adequacy of current tests for predicting the sooting tendency of fuels will be evaluated during this study.

l. Probe and Optical Measurement of Carbon Monoxide. In a recent study performed for AFESC and the Air Force Aero Propulsion Laboratory, investigators at the Arnold Engineering Development Center (AEDC) found widely different results for carbon monoxide (CO) in the exhaust of a gas turbine combustor using three different extractive probe designs: an expansion probe, a dilution probe, and a constant diameter probe. To shed light on this discrepancy, an in-situ optical measurement was performed using a gas filter correlation spectrometer built for this purpose by AEDC personnel. Unfortunately, poor signal to noise ratios due to flame radiation, limited operation to idle conditions. Under these conditions the optical technique agreed with measurements obtained with an orifice (expansion) type probe. However, in the earlier study the three probe designs also agreed at idle conditions. Only at higher power settings did they diverge, with the dilution and expansion probes yielding CO results in order of magnitude higher than the constant diameter probe.

m. Interagency Investigation of NO. In a number of studies investigators at AEDC have reported discrepancies between optical and probe extractive measurements of NO in gas turbine combustor exhausts. As a result, a joint effort was undertaken by the FAA, EPA, NASA, Navy, and AFESC to determine whether the optical or probe results were correct and to investigate the source of the disagreement. The contractor, United Technology Research Center, used three different calibration techniques to

validate the optical measurements throughout the temperature regime of interest: a static gas cell at room temperature, a flowing gas heater up to 900K and a hydrogen flat flame for temperatures up to 1700K. The dynamic methods were needed due to the instability of NO at high temperatures. Several errors in the AEDC computer model used with the optical technique were identified and corrected. Following this, the optical and probe results showed good agreement on three combustion systems of increasing complexity ranging from a methane flat flame to an operational combustor can. It was concluded that the corrected optical technique provides accurate measurements of NO; and that probe extraction is also a reliable method if carefully done with a cooled probe designed to provide a "rapid quench" of the sample.

n. Transformation of NO_x in Sampling Probes. For several years, Dr G. S. Samuelsen of the University of California, Irvine, has been investigating the conditions under which oxides of nitrogen might be transformed in sample lines used for combustion diagnostic measurements. Currently, AFESC is funding an amplification of the ongoing AFOSR grant supporting this research in order to specifically address the conditions typically found during sampling of gas turbine engine exhaust. Included in the study are the effects of probe material, previous probe history, exhaust gas composition, contact time, and sampling pressure. Conditions both at the probe tip and in the sample line are being studied in parallel experiments. Results to date indicate that reduction of NO_x including total destruction, can take place under the right conditions. Stainless steel probes provide a more reactive surface than quartz, and reducing materials, such as hydrogen and alkenes, promote such effects.

o. Measurement of Aircraft Exhaust Composition Using Long Path Infrared Spectroscopy. To demonstrate the potential of non-contact optical techniques for monitoring aircraft exhaust emissions, AFESC invited Dr William F. Herget, chief of the EPA Special Techniques Group, to bring his Remote Optical Sensing of Emissions (ROSE) system to Tyndall Air Force Base. The ROSE system consists of a specially instrumented van, including a Fourier transform infrared spectrometer and associated optics which permit measurements over an atmospheric path up to several kilometers. Measurements were performed of the exhaust from an Air Force F-101 "Voodoo" jet aircraft at idle, full power, and afterburner power settings. Species identified include NO, CO, CO_2, acetylene, ethylene, and formaldehyde. A continuum absorption due to hydrocarbons was also observed in the 2800-3100 wave number spectral region. Agreement between the spectroscopically determined species concentrations and typical values obtained using extractive probes (in different studies) was good.

p. Measurement of Hydrocarbons by Gas Correlation Spectroscopy. The greatest difficulty in developing an optical

technique for measuring total hydrocarbon concentrations in aircraft exhaust is the complex mixture of hydrocarbon species emitted. To overcome this difficulty AFESC joined with EPA to sponsor a study by Dr Darrell Burch of the Aeronutronic Division of Ford Aerospace and Communication Corporation to investigate the application of gas correlation spectroscopy to mixtures of hydrocarbons. A highly flexible gas correlation instrument was modified to perform measurements using a variety of hydrocarbons. The response of the instrument will be used to evaluate the potential of the technique to provide a non-intrusive alternative to the current FID method. One possible wavelength region is 3.0 to 3.5 microns, where most hydrocarbons have an absorption due to C-H bond stretching. Although such a method would probably require separate calibration for each given type of source (e.g., aircraft emissions versus evaporative storage losses) its use would still be advantageous in cases where probe extraction was impractical.

q. Passive, Single Ended Measurement of CO. Due to the high temperature of aircraft engine exhaust, it should be possible to obtain non-contact optical measurements of exhaust species in emission. That is, using the hot exhaust itself as a source of energy, a passive gas filter correlation instrument could monitor effluent concentrations without the need to align separate light source. To determine the feasibility of such a system, AFESC joined with the EPA to sponsor a study by Dr Lucien Chaney of the University of Michigan. Using two existing EPA long path instruments originally designed for double ended use, Dr Chaney will investigate the important parameters involved in single ended operation including source temperature, background levels, and non-spectral radiation interference. The study will emphasize use for CO and SO_2.

r. Differential Absorption LIDAR for Measurement of Aircraft Emissions. Capitalizing on MIT Lincoln Laboratory's expertise in laser technology, AFESC is sponsoring a research effort to extend the state-of-the-art in the application of lasers to environmental monitoring. A high repetition rate miniature CO_2 TEA laser developed by Lincoln Laboratory has been integrated with the necessary optics and signal processing electronics to form a differential absorption LIDAR system. This system uses the difference in reflected laser return at wavelengths on and off an absorption feature of a given pollutant to determine a path average concentration. Measurements of NO and CO in the 5 micron region (using a non-linear doubling crystal) have been demonstrated over kilometer long atmospheric paths as well as for point sources including the exhaust from an Air Force turbine engine powered helicopter. Further studies will attempt to measure ethylene and the hydrazine based propellants in the 10 micron region. Eventual incorporation of Lincoln Laboratory's new $Ni:MgF_2$ laser technology should provide sufficient power to

obtain range resolved measurements using return from the natural aerosol.

s. Alternative Fuels Environmental Studies.

(1) Atmospheric Chemistry. As a part of a larger study including conventional jet fuels and cruise missile fuels, shale oil derived JP-4, JP-5 and JP-8 will be investigated as to their potential atmospheric reactivity. Areas of study will include photochemical reactions, reaction product determinations and the effect of different reaction conditions on these processes.

(2) Aqueous Chemistry. Shale oil derived JP-4, JP-5, and JP-8 will be studied in freshwater, saltwater, and distilled water solutions. Components of the fuels will be identified and quantitated and solubilities measured in the different aqueous media. Effects of aeration, ultra-violet light, and agitation on solubility will be determined and any decomposition/transformation species identified.

t. Combustion Characteristics of Refuse-Derived Fuel (RDF) and RDF:Coal Blends. This investigation is being conducted by the U.S. Army Construction Engineering Research Laboratory (CERL) under funding provided by the Navy and AFESC to determine the combustion kinetics of fuel samples containing RDF mixed in varying proportions with Midwest bituminous coal. Investigative work is being carried out in an 18-inch diameter stationary bed thermogravimetric facility equipped with a dense array of thermal sensors, an on-line gas chromatograph, and a 2-watt argon ion backscattering laser doppler anemometer. Results of the experiments will be used to design a long-term full-scale RDF:coal experiment in an Air Force central heating or power plant as part of the facilities energy R&D program in FY80-81.

u. Cofiring Refuse-Derived Fuel (RDF) and Coal. This experiment is being conductged at Wright-Patterson AFB where pelleted RDF is being blended with coal and cofired in a large central power plant. A major focus of the R&D aspects of this fuel substitution effort is on furnace and heat exchanger performance changes as the fraction of RDF increases, and on determining limiting RDF substitution ratios for desired steam generating capacity. The experiment will continue for 18 months, will include Navy and Army resources, and will be jointly led by Air Force logistics Command and AFESC personnel.

v. Coal and Oil Mixtures. This FY80 investigation will be performed by a contractor yet to be determined. The objective of the work, which will be funded by AFESC, is to determine the technical potential of converting Air Force gas and oil-fired boilers and diesels to using various alternative

solid fuels mixed with oil. Alternative fuels to be considered include refuse-derived fuel, biomass, coal, and thixotropic materials. The investigation will consider not only fuel preparation and firing technology, but also maintenance of reliable continuous mobilization-level combustor performance. A follow-on full-scale, thoroughly monitored demonstration of promising concepts is being planned.

Ionic Mechanisms of Carbon Formation in Flames

Contract No. F49620-77-C-0029

H.F. Calcote and D.B. Olson

AeroChem Research Laboratories, Inc.

P.O. Box 12, Princeton, NJ 08540

The formation of soot in the combustion of hydrocarbon fuels is a problem which has received much attention, yet the basic physical and chemical processes controlling the phenomena remain unknown. The practicality of the problem is widely recognized and it is of direct relevance to numerous Air Force missions.

It is the objective of this program to further the understanding of these phenomena by providing a chemical mechanism which can be used in model predictions to solve practical problems. The hypothesis which the experimental program seeks to test is that ions produced via chemi-ionization serve as nuclei for the formation of soot particles. Evidence has accumulated which indicates that the normal neutral/radical chemical processes of hydrocarbon combustion reach a bottleneck where the thermochemistry and kinetics prevent the production of larger and larger molecules on the pathway of soot formation. The ion chemistry, normally only a minor feature of a combustion system, is proposed as a route whereby rapid ion-molecular kinetics, rapid ion structural rearrangements, and favorable thermochemistry lead to rapid growth of large polycyclic ions and particle formation.

These objectives are being pursued by mass spectrometric measurements of ion profiles in low pressure premixed flat flames of several representative fuels. The majority of the results have been obtained with acetylene/oxygen and benzene/oxygen flames at 15 Torr at equivalence ratios above and below the critical equivalence ratio for soot formation. Detailed individual ion species profiles were measured up to mass 300 and profiles of all ions as a group larger than mass 300 were measured.

The ion profiles of acetylene and benzene flames exhibit many similarities and some distinct differences. The basic trend is for $C_3H_3^+$ to dominate in rich non-sooting flames with larger ions (for example $C_5H_5^+$, $C_7H_5^+$, and $C_{13}H_9^+$) becoming increasingly important as the soot point is approached. As a strongly sooting (yellow-orange) flame is approached by increasing the equivalence ratio, these ions quickly disappear and are replaced by large concentrations of ions with mass > 300. Peculiar to benzene is the appearance in the early region of the flame of oxygenated aromatic ions, e.g., masses 95, 109, 119, 131, etc., corresponding to:

$C_6H_7O^+$, $C_7H_9O^+$, $C_8H_7O^+$, and $C_9H_7O^+$. The neutral precursor of these ions is probably C_6H_6O which has been observed by Bittner and Howard in benzene flames at significant concentrations. Later in the benzene flame the ion spectrum becomes very similar to that observed in acetylene flames. A unique observation is that, although benzene and acetylene soot at very different equivalence ratios, this sooting occurs when the large positive ion concentration (mass > 300 and probably less than ≈ 2,000) reaches the same value for both flames. It seems significant that the location of these mass > 300 ions corresponds with the location of a group of neutral species identified earlier by Homann and Wagner as "soot precursors". These workers identified these precursor species only as reactive polycyclic aromatic hydrocarbons probably with side chains and containing more hydrogens than aromatics.

A mechanism has been developed for acetylene flames which accounts for the observed ion spectrum including the relative species concentrations. The mechanism simply considers the ion-molecule addition reactions $A^+ + B = C^+$ where A^+ is $C_3H_3^+$ and larger ions, and B = C_2H_2, C_4H_2, and C_2H, the reactive neutral species of highest concentration. Only exothermic reactions are allowed. The $C_3H_3^+$ is assumed to be produced by the usual chemi-ionization reactions: CH + O and CH* + C_2H_2. Simple calculations give remarkable qualitative correspondence with experimental observations. The benzene mechanism has not been considered in detail since the combustion chemistry is not well known and therefore the neutral "monomers" for addition to the ions are unknown. Brief consideration has been made of the possible routes for production of species unique to benzene. Reasonable results are obtained using C_6H_6O as a neutral to which $C_3H_3^+$ and other ions add (sometimes eliminating H_2 to obtain structures of higher resonance stability).

A unique feature appears in the ion concentration profiles through the flame upon approach to the sooting point. The ion concentrations which normally decrease beyond the blue-green flame zone are observed to increase again and a dual peak profile of ion concentration vs. distance results. This behavior is obtained for ions of mass larger than about 89. It appears in both acetylene and benzene and is strongest in the profiles of the mass > 300 species. The reasons for this phenomenon are not understood. One possible explanation assumes a change in the identity of the negative charge carrier from electrons in the non-sooting flames to large negative ions in the sooting regions of richer flames. The reduced mobility of these heavy negative ions would result in reduced recombination coefficients and therefore reduced loss terms for the positive ions. Another explanation would require an additional source of chemi-ions; thermal ionization cannot explain the results. We are currently preparing to measure the negative ion profiles in these same flame systems to help answer these questions.

Additional future work is planned to measure the ion profiles to much larger masses. By following the species to mass 5000 we hope to be able to conclusively determine the role of ions in soot formation. Construction of apparatus to accomplish this is under way.

MECHANISMS OF EXHAUST POLLUTANT AND PLUME FORMATION IN CONTINUOUS COMBUSTION
AFOSR-78-3586

G. S. Samuelsen

UCI Combustion Laboratory
School of Engineering
University of California, Irvine

INTRODUCTION

The present analytical and experimental investigation is designed to clarify the relative influence of the mechanisms responsible for pollutant production in continuous combustion, develop and evaluate predictive methods for characterizing reacting flows, and assess experimental errors associated with sampling oxides of nitrogen. The research program encompasses studies of the physical and chemical processes contributing to pollutant and plume formation in jet engine continuous combustors. The results of the research will aid in establishing guidelines and techniques for reducing adverse environmental effects and controlling plume signatures in present day and advanced jet engine combustors by control and modification of the combustion dynamic processes.

Combustion experiments are being conducted with both nonreacting and reacting laboratory combustors under conditions simulating the basic flow characteristics of gas turbine engines. In addition, theoretically predicted profiles of the flow properties are being compared with experimentally determined profiles to evaluate the predictive methods used to solve the governing differential equations and the associated models of turbulence and chemical kinetics for reacting flows. Deficiencies in present models are being identified and used to refine the predictive models with the goal of accurately predicting the formation of combustion-generated pollutants.

Sampling experiments are being conducted with simulated combustion products at concentrations representative of primary and secondary zones of gas turbine combustors, and exhaust planes of gas turbine engines. Conditions for which changes occur in oxides of nitrogen concentration and composition during sample extraction and sample transport are being identified and used to refine the experimental methods with the goal of accurately measuring combustion-generated pollutants.

RESULTS

The evaluation and development of predictive methods have emphasized the performance of predictive methods in describing mass and momentum transport in recirculating flows in the absence of reaction. The turbulent flowfield of an atmospheric backmixed combustor has served

as the vehicle for examination. The configuration is a turbulent pipe flow with an on-axis jet opposing the main flow. Mass transfer is evaluated by introducing a tracer species (carbon monoxide) through the jet and observing the axial and radial mass transport. Momentum transport is evaluated by comparison of experimentally measured profiles of velocity and turbulent kinetic energy to those predicted. Thermal transport is evaluated by preferentially heating the jet and comparing the axial and radial measured profiles of the mean and fluctuating component of temperature to those predicted. It has been shown earlier that the predicted transport characteristics are strongly influenced by (1) the specification of the coefficients in the source and sink terms of the turbulence energy dissipation rate equation, (2) the specification of turbulence kinetic energy at the jet inlet, and (3) the specification of boundary conditions for the eddy dissipation rate in the vicinity of the recirculation zone. The temperature data have further demonstrated a need for a closer examination of the ε equation and the assumption of constant Prandtl and Schmidt numbers. In addition to the primary combustor, a water analog of the flow has been constructed and used to obtain spatially resolved measurements of velocity and turbulence intensity using laser doppler anemometry. Results consistent with the gaseous flow are found, with comparable levels of turbulence intensity and jet penetration. The water analog is designed to facilitate flow visualization and promote a full description of the flowfield aerodynamics; high speed cinematography is in progress.

The reacting flow studies have focused on internal flowfield measurements of species composition and temperature. The opposed-jet combustor has been operated for a range of main and jet stream velocities and equivalence ratios to assess the effect of recirculating zone mixing and intensity on pollutant formation. It has been demonstrated that the combustor can be tailored (enriched jet, lean mainstream) to reduce NO_x emission by a factor of 10. At the flame front, NO_2 is the dominant NO_x species measured, the presence of which is attributed to the rapid mixing between the hot combustion products and the relatively cold, oxygen-enriched reactants. The data also provide an experimental base against which predictive modeling can be tested.

Testing of an alternative combustor geometry is in progress. The combustor comprises a solid cylinder aligned symmetrically within a cylindrical tube. Flow through the annulus dumps over the face of the solid center body cylinder. Operation can be either premixed or nonpremixed. The annular jet in the case of premixed is a mixture of fuel and oxidant. In the case of nonpremixed operation, the annular jet is air with fuel injected through either an axially positioned fuel tube or nozzle located on the face of the center body. Optimization studies have included both swirl and nonswirl in the annular jet. The performance is found to be highly sensitive to mixing scale in the annular jet.

The sampling experiments have addressed the effect of sample line surface condition on the change to nitrogen oxides composition and concentration during transport. Stainless steel tubes (¼-inch O.D.) that are pre-oxided or pre-reduced are found to modify the chemical change, the extent of which depends on the conditions under which preconditioning occurs.

FUNDAMENTAL COMBUSTION STUDIES

RELATED TO AIR-BREATHING PROPULSION

F. A. Williams

Professor of Aerospace Engineering

Department of Applied Mechanics and Engineering Sciences

University of California, San Diego

La Jolla, California 92093

This research is directed toward developing basic information that is relevant to continuing problems in air-breathing combustion, specifically to improvement of efficiencies, to reduction of undesired emissions and to increase in accuracies of design methods. Recently, the work has been focused mainly on turbulent combustion of gases. Specifically, new theoretical results have been obtained on turbulent flame speeds, which are useful in designing combustion chambers for maximum efficiencies.

Particular attention has been given to the extension of a previously developed theory for the structure and propagation velocity of premixed flames in turbulent flows having scales large compared with the laminar-flame thickness. The molecular coefficients of diffusion for heat and reactants were allowed to differ by an amount of the order of the reciprocal of the nondimensional activation-temperature, one of two expansion parameters in the analysis. Velocity fluctuations were found to introduce differential fluctuations in flame temperature which depend on the ratio of diffusivities, the Lewis number. The consequent modification to the turbulent flame-speed was calculated by carrying the analysis to second order in the ratio of the laminar-flame thickness to the turbulence scale. It was found that for a Lewis number different from unity there exists an additive contribution to the flame speed which is proportional to the average rate of dissipation of kinetic energy of turbulence. This contribution arises from influences of flame stretch.

At this stage, three specific influences on the turbulent flame speed have been identified. When streamwise and transverse turbulent fluctuations are comparable in magnitude, the largest contribution, within the context of a small-gradient expansion, is that of wrinkling of the laminar flame sheet. The associated area increase of the reaction sheet of the laminar flame causes the turbulent flame speed to exceed the laminar flame speed. Previously a formula providing this area increase, and hence the turbulent flame speed, in terms of statistical properties of the up-

stream turbulent field had been derived for situations in which the departure of the reaction surface from a planar shape was small. In new work, through a somewhat different method of performing the perturbation expansions, a modification to the formula for the area increase was derived which allows for large departures of the reaction surface from a planar configuration. Thus, calculations of the flame-wrinkling effect on turbulent flame propagation can now be made for larger extents of wrinkling.

The second largest contribution is the flame-stretch effect identified above. It has long been known that laminar flame-stretch influences turbulent flame propagation, but the nature of that influence has not been known. The new analysis that was developed remains valid only if the difference of the Lewis number from unity is small enough to exclude cellular-flame types of inherent instabilities. Under this restriction, the flame-stretch effect was found to provide an additional increase in the turbulent flame speed, beyond that due to flame wrinkling, provided that the molecular diffusivity of the reactant exceeds that of heat. If the diffusivity of heat is the larger, then the flame-stretch effect tends to decrease the turbulent flame speed. The new flame-speed formula that has been derived enables these stretch effects to be calculated explicitly in terms of statistical properties of the upstream turbulence. Sufficiently large stretch is known to produce disruption of the reaction surface if the Lewis number differs from unity. Thus, this aspect of the analysis potentially allows improved estimates to be made of the limits of validity of the analysis.

The third largest contribution to the departure of the turbulent flame speed from the laminar flame speed is the influence of flame curvature. The effect of curvature on laminar flames is roughly similar to that of stretch. In the analysis that was developed, the mean-square value of a linear combination of the curvature and stretch effects appears in the formula for the turbulent flame speed. Thus, the influence of reaction-sheet curvature on the turbulent flame speed is qualitatively similar to the stretch effect, but generally smaller in magnitude.

The work has revealed a number of aspects of the dynamics of laminar flames in turbulent flows, including the tendency toward instability at the critical Lewis number. It is hoped that future study will provide results on turbulent flame speed valid in regions of instability and disruption of wrinkled laminar flames.

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ALTERNATIVE AVIATION TURBINE ENGINE FUELS AND THEIR COMBUSTION CHARACTERISTICS

C. L. Delaney, H. R. Lander, T. A. Jackson, C. R. Martel

AIR FORCE AERO PROPULSION LABORATORY, FUELS BRANCH
WRIGHT-PATTERSON AIR FORCE BASE, OHIO 45433

As the Air Force agency responsible for the research and development of aviation turbine fuels (jet fuels), the Air Force Aero Propulsion Laboratory is addressing jet fuel cost and availability problem by encouraging the development and production of fuels from nonpetroleum sources and by broadening existing fuel specifications to permit more jet fuel to be made from petroleum. Specific research and development programs include: (1) investigation of the feasibility of making jet fuels from oil shale, coal, and other nonpetroleum sources (completed), (2) conduct combustor/turbine component tests to determine the effects of various fuel properties and characteristics on engine performance and durability (underway),(3) examine various candidate shale oil processing techniques to obtain information on fuel costs, availability, properties, and problems (underway), (4) conduct tradeoff studies of fuel processing costs, fuel properties, and fuel effects on aircraft and engine performance and durability so as to minimize life cycle costs (underway), and (5) conduct flight tests and qualification tests of broadened specification fuels and fuels from nonpetroleum sources.

The AFAPL combustion/turbine programs consist of component rig, and engine tests to quantify the relationships between fuel properties and the performance/durability of the combustor and turbine hardware of representative aircraft gas turbine engines. Fuel properties of primary concern include hydrogen content, aromatics types, distillation range, distillation endpoint, and viscosity - fuel properties that are all interrelated. In addition, basic research combustor programs are underway that will be discussed in detail at a later time.

Combustor programs that have already been completed include the in-house tests of a T-56 combustor and the contractor performed tests of the F-101, J-79, TF-41, and a high Mach experimental combustor. Thirteen (13) different fuels were tested ranging from JP-4 to number 2 diesel fuel. Fuel hydrogen contents varied from 12% to 14.5% by weight. These tests identified the fuel hydrogen content as the primary fuel property affecting combustor durability. Fuel volatility and viscosity were found to control high altitude relight and low temperature starting.

Programs currently underway include combustor and turbine component rig tests and limited full engine tests of the PT-6, JT-15D, J-57, J-79, J-85, F-100, and TF-39 engines using up to six selected test fuels. Also a program is being initiated to determine the effects of fuel properties on afterburner performance for the J-79, J-85, F-100 and TF-30 engines.

Concurrent efforts are underway to obtain flight test quantities of oil shale derived jet fuels. Flight tests of oil shale derived fuel meeting current JP-4 specifications may be possible by 1982-83, and operational validation tests of oil shale JP-4 could occur as early as 1983-84. The first broadened fuel specification is anticipated to be ready by 1987.

Emergency fuels was a topic specifically requested to be addressed in this presentation. Air Force Technical Order 42B1-1-14 lists specified fuels, alternate fuels, and emergency fuels for all aircraft. Specified fuels are fuels with which aircraft were designed to operate. Alternate fuels may be used continually but can reduce mission capabilities. (Note that within the Air Force 'alternate fuels' has a special meaning.) Emergency fuels are for one time use only and can reduce both mission capabilities and engine durability. As an example, for the KC-135 the specified fuel is JP-4. Alternate fuels are JP-5, JP-8, Jet B, Jet A, and Jet A-1. The emergency fuel is aviation gasoline (AvGas). The higher freezing points and degraded high altitude relight and low temperature starting performance of the alternate fuels can obviously affect mission capabilities. With the emergency fuel, AvGas, excessive boiloff losses would affect range, vapor lock is possible, and the tetraethyl lead may affect engine hot section durability.

The only other fuels that could possibly be considered for emergency use in most aviation turbine engine powered aircraft would be motor gasolines (mogas) and diesel fuel. With mogas the volatility problems would be even more severe than with AvGas. With diesel fuel the freeze point and engine starting/relight problems would be much more severe than with kerosene fuels such as Jet A, A-1, JP-5, and JP-8. In summary, aviation turbine fuels for existing aircraft cannot have volatilities significantly greater than JP-4 or significantly less than JP-5 and JP-8 fuels without seriously affecting aircraft performance and safety. Similarly, the freezing point of fuels cannot be greater than -40°C (-40°F) without seriously compromising mission capabilities and flight safety.

COMBUSTION PHENOMENA ASSOCIATED WITH ADVANCED FUELS FOR VOLUME LIMITED PROPULSION SYSTEMS

A. F. Bopp and J. R. McCoy

Air Force Aero Propulsion Laboratory

Wright-Patterson Air Force Base, Ohio 45433

Over the past ten years the Air Force has developed a series of fuels for use in volume limited missile systems. These fuels are JP-9, JP-10, RJ-5, and RJ-6. Like JP-4, these fuels are liquid hydrocarbons but possess a much greater mass density and higher C:H ratio. Unlike the distillate fuels which contain literally hundreds of compounds, they contain very few different chemical species. This limited number of chemical species, hench range of chemical properties, make these fuels prime candidates for basic research into combustion chemistry.

In addition to these liquid hydrocarbons, the Aero Propulsion Laboratory is currently developing a carbon slurry for use as the propellant in cruise missile systems. These fuels contain submicron size carbon particles suspended in JP-10 or RJ-6. The combustion of these heterogeneous systems is expected to be quite complex. After volatilization of the liquid carrier, the hydrocarbon vapor combusts rapidly compared to the solid carbon fraction. The onset and rate of particulate combustion in relation to liquid combustion are prime areas of interest in our programs. Slurried fuels employing solid boron are also being contemplated by the Air Force. The uncertainties associated with carbon combustion will be magnified by lack of reaction rate data for boron.

CARBON SLURRY FUEL COMBUSTION
(AFAPL Contract No. F33615-78-C-2025)

W. S. Blazowski and D. C. Rigano

Exxon Research and Engineering Company
P. O. Box 45
Linden, New Jersey 07036

Background

Improving the range and payload of modern and future cruise missile systems will require the development of fuels with increased volumetric energy content. Air Force and Navy-sponsored research has resulted in impressive advances in fuel Btu content over the past 20-30 years. Liquid fuels including exo-tetrahydrodi(cyclopentadiene), now called JP-10, have been developed. Further improvements have been made in these bridged-ring saturated hydrocarbons and a series of materials allowing energy contents up to 160,000 Btu/gal. are currently available.

It now appears that a practical limit is being approached for entirely liquid fuels and further improvements in range through innovation in fuel composition will require the use of stable dispersions of carbon or boron in a liquid, commonly referred to as slurry fuels. The Air Force initiated a program with Exxon Research and Engineering Company (ER&E) in late 1978 to develop a solid-carbon-containing fuel which will have a volumetric energy content of 180,000 Btu/gal.

Results of Exploratory Program

Combustion evaluations utilized a new stirred reactor capable of burning both liquid and multi-phase carbon slurry fuel. Previously, well-stirred combustors were designed only to operate with gaseous fuel. The Liquid Fuel Jet Stirred Combustor (LFJSC) incorporates both a recirculation region typical of the primary zone and a turbulent non-recirculating zone typical of the secondary zone of a gas turbine. The LFJSC can be operated at varying equivalence ratios, temperatures and residence times.

Experience gained from the shakedown operation of the LFJSC has shown that fuel injector design for carbon slurry fuels will be a problem and clearly indicates a need for increased attention to this area in the future. Two critical design problems have been identified: (1) excessive heating of the liquid portion of the slurry fuel in fuel lines and nozzles must be avoided, and (2) the injector must be carefully designed to prevent unburned carbon from coming close to combustor walls and depositing.

Combustion performance testing indicated that carbon burnout efficiencies greater than 90% are achievable with 300 mμ particles

in residence times down to 4 ms. An insensitivity of carbon burnout to residence time was noted. This suggests that a portion of the 300 mμ particles formed large agglomerates when formulated or during vaporization within the combustor. These larger particles could not be consumed during the range of times available, resulting in the noted burnout insensitivity. The data also indicate that burnout is a function of mixture conditions and that the optimum equivalence ratio is approximately 0.8. Since conventional combustors do not provide substantial time at this mixture condition, combustor redesign to accommodate carbon slurry fuels may be needed. Limited tests indicate that smaller carbon particle size may result in improved carbon burnout.

Experiments were conducted to determine if homogeneous catalysts (i.e. the addition of a soluble catalytic material to the liquid portion of the carbon slurry fuel) would accelerate the burnout of carbon particles. Results to date show that manganese, iron, or lead-based homogeneous catalysts will not significantly accelerate carbon particle burnout and imply that heterogeneous catalysts should be investigated. In the heterogeneous approach, small levels of active solid catalyst will be added directly to the surface of the carbon particles before the carbon and liquid are mixed to form the slurry fuel.

Research Needs

Carbon slurry combustion is one topic on which research can make a major contribution to a near-term development. Contributions can be in three major areas:

- Agglomeration during droplet volatilization may be a serious problem. The slurry enters the combustion system as liquid droplets containing approximately 60% by weight of very small particle size carbon. Vaporization of the slurry droplet must be such that the carbon particles enter the gas phase individually or in small groups. If gross agglomeration occurred--all the liquid is removed without causing the carbon particles to disperse-- a large mass of carbon would remain. The burning time of such a large diameter particle would be unacceptably long. It is important that an understanding of the slurry droplet vaporization process be developed so that approaches which minimize agglomeration may be pursued.

- As use of carbon slurry fuels approaches the development stage, analytical models can be used to make predictions, correlate data, and provide design guidance. Such capability, which could at first be modular combinations of

stirred reactors, plug flows, and shear layer mixing regions, has not yet been developed for multi-phase fuels and is a definite need.

- The overall state of knowledge of carbon particle and soot oxidation leaves much to be desired. A study of the literature, including measurements of soot and various types of carbon particles, reveals an unusually broad range of burning rates. The models referred to above will require more accurate oxidation kinetic rate information from fundamental experiments (e.g. shock tube, flat flame) for the actual carbon types being utilized.

EPA SUPPORTED RESEARCH, DEVELOPMENT TRENDS AND RESEARCH NEEDS IN AIR-BREATHING COMBUSTION

S. Lanier
EPA

Abstract not received

AGENDA

1 February 1980

Friday AM

FRIDAY

AGENDA

1 February 1980

Friday PM

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APPLICATIONS OF ADVANCED DIAGNOSTIC TECHNIQUES TO MEASUREMENT OF PARAMETERS IN AIR-BREATHING PROPULSION SYSTEMS

D. L. Hartley

Combustion Sciences Department
Sandia Laboratories
Livermore, CA 94055

Optical diagnostic techniques, including laser fluorescence, laser doppler anemometry, laser Raman scattering, Rayleigh and Mie scattering are being used at Sandia to study a variety of combustion research problems relevant to air breathing propulsion systems.

For fundamental flame analysis, fluorescence is being used to probe ambient and low pressure systems for measurement of minor radical species; laser Raman scattering is used to measure concentrations and temperatures in laminar and turbulent diffusion flames; Rayleigh scattering is used to measure temperature fluctuations; LDA is used to map velocity fields.

For air-breathing piston engine combustion studies these techniques are being applied to Sandia to measure the transient fluid mechanics and chemical processes.

For solid-fuel fired gas turbine combustion systems these techniques are being modified to measure concentrations and temperatures in particle-laden flows and to measure the particulate size and number density.

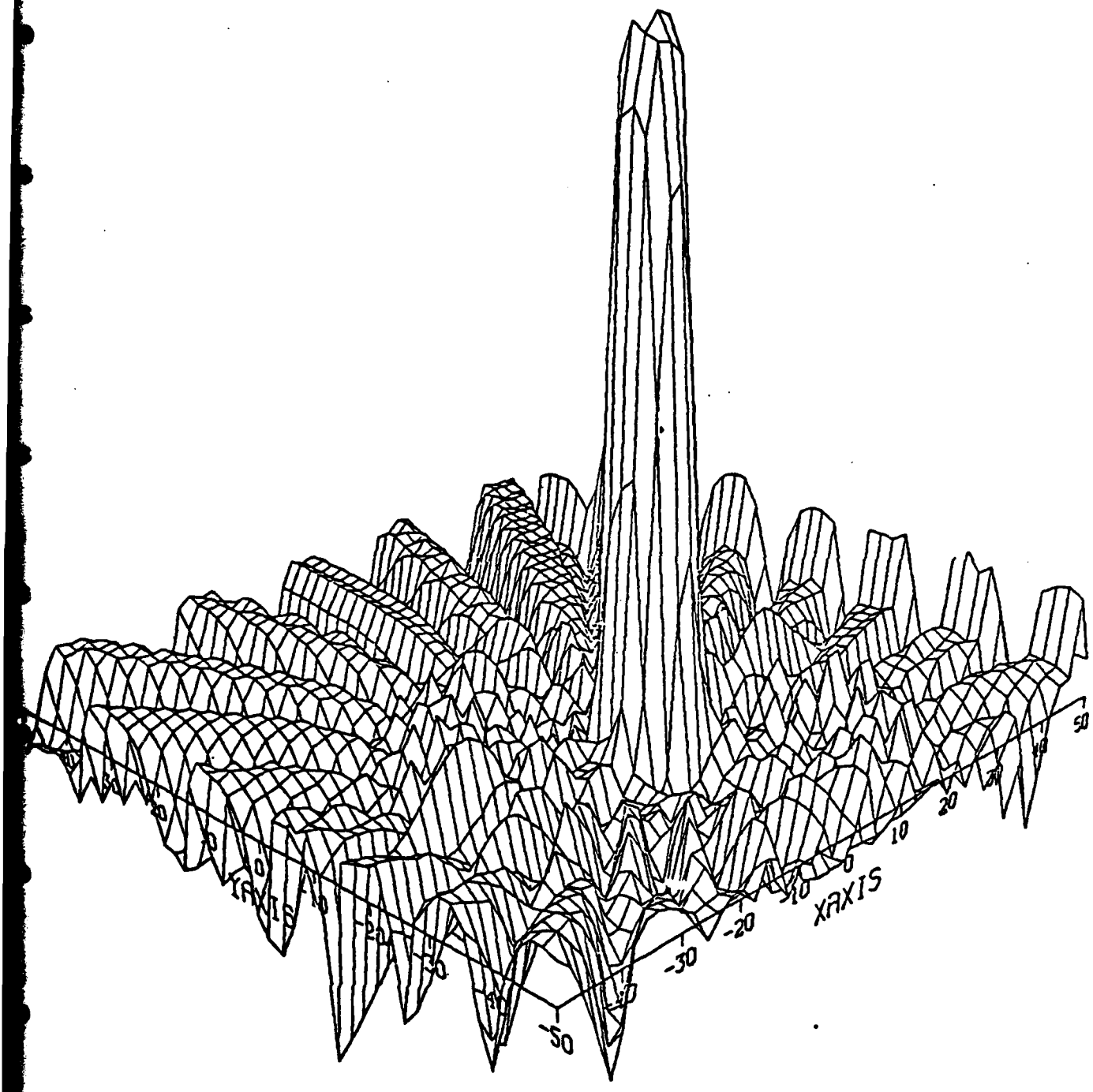
MULTIANGULAR ABSORPTION DIAGNOSTICS IN COMBUSTION

R. Goulard and P. J. Emmerman
School of Engineering and Applied Science
The George Washington University
Washington, D. C. 20052

Absorption techniques are being applied to three-dimensional combustion diagnostics. Convolution Fourier transforms and iterative algorithms have already been proven in x-ray absorption tomography and interferometric applications. They are currently tested and compared on typical pollutant and radical concentrations as they appear in flames or exhausts. The effect of the number of scans is analyzed for parallel beams.

A trade-off exists between accuracy and the number of viewing angles. A five-angle procedure gives 10% accuracy with a moderately filtered convolution algorithm. An experiment feasibility study shows that near time-continuous three-dimensional maps of low concentration (1 ppm) can be obtained at repetition rates up to 10 KHz.

The potential of this method was demonstrated in the laboratory. A diluted methane jet was observed at several sections along its axis. Steady two-dimensional profiles were reconstructed from the absorption scans effected from six and twelve angles. The theoretically predicted dependence of the accuracy on the number of observation angles was verified. Real time experiments are now being prepared.



Reconstruction of methane jet cross section for twelve angle case

THEORETICAL MODELING AND EXPERIMENTAL INVESTIGATIONS OF REACTING FLOWS IN PRACTICAL AIR-BREATHING ENGINE COMBUSTION ENVIRONMENT UTILIZING ADVANCED DIAGNOSTIC TECHNIQUES

W. M. Roquemore, R. P. Bradley, J. S. Stutrud and C. M. Reeves
Air Force Aero Propulsion Laboratory
Wright-Patterson Air Force Base, Ohio 45433

L. Krishnamurthy
University of Dayton Research Institute
Dayton, Ohio 45469

A program is in progress at the Air Force Aero Propulsion Laboratory (AFAPL) to evaluate combustor models in environments which simulate many of the features in gas-turbine combustors. This program involves the selection and evaluation of appropriate diagnostic techniques for making time-averaged and time-resolved point measurements of velocity, temperature, and major species concentration in simulated, practical combustion environments. The most promising diagnostic techniques will be used to collect data for combustor-modeling evaluation and development. A description of this program is presented. Also, a special bluff-body combustor has been developed for the program. To facilitate modeling studies and the evaluation of diagnostic techniques, the combustor is designed with simple axisymmetric geometry and easy measurement access to the reaction zone. The combustor configuration consists of a 14 cm diameter shrouded disk centered in a 25.4 cm diameter duct with gaseous propane injection at the center of the disk through a 4.8 mm diameter tube. The combustor is operated at atmospheric pressure and room air inlet temperatures and burns gaseous propane. Measurements of flame lengths and the rich and lean blow-off limits are presented. Combustion inefficiencies are presented at selected air and fuel flow rates. For a constant air flow rate, the combustion inefficiency passes through a minimum as the fuel flow rate increases. Photographs show that the shape of the flame changes dramatically as the air and fuel flow rates are varied. The changes in flame structure and the changes in inefficiency are believed to be due to the influence of the fuel jet on the recirculation zone. Qualitative descriptions of the flowfields believed to be responsible for the observed changes are given.

CARS MEASUREMENTS IN SIMULATED AIR-BREATHING ENGINE COMBUSTION ENVIRONMENTS

G. L. Switzer and L. P. Goss
Systems Research Laboratories, Inc.
Dayton, Ohio 45440

P. W. Schreiber
Air Force Aero Propulsion Laboratory
Wright-Patterson Air Force Base, Ohio 45433

As part of an AFAPL sponsored program, coherent anti-Stokes Raman spectroscopy is being investigated as a method for collecting temperature and species concentraction data for evaluating combustor models. Results of CARS experiments performed in a combustor which produces a bluff-body-stabilized flame having recirculating flow characteristics similar to those in many practical combustion systems are presented. These results were obtained from the following CARS measurements with gaseous propane used as the fuel: determination of temperature profiles in the flame based upon the analysis of the scanned N_2 spectra (time-averaged spectra), and the mapping of the concentration of N_2 and O_2 based upon the broad-band integration of all Q-branch lines using a single laser pulse. Presented also are: (a) comparison of CARS temperature data and those from a thermocouple taken at the same locations in the combustor, (b) comparison of CARS concentration data for O_2 and those obtained with a gas sampling probe, and (c) comparison of temperature data obtained by single-pulse CARS and by the sodium line-reversal method. In addition, preliminary results obtained experiments using the liquid fuels JP-4 and shale-oil-derived JP-8 are also reported. The results obtained to date indicate that with the CARS technique spatially and temporally resolved measurements of species concentration and temperature can be made in the reacting zone of large-scale combustors using gaseous or liquid fuel.

INVESTIGATION OF LASER INDUCED FLUORESCENCE SPECTROSCOPY FOR MAKING IN-SITU SPECIES CONCENTRATION AND TEMPERATURE MEASUREMENTS IN TURBULENT COMBUSTION FLOWS AFOSR-77-3357

John W. Daily

University of California
Department of Mechanical Engineering
Berkeley, California 94720

The study of reacting gas flows has traditionally been limited by a lack of experimental data. The measurement of temperatures and species concentrations in complex flames with sufficient spacial and time resolution would be especially desirable. Under AFOSR Grant 77-3357 we have been investigating the application of saturated Laser Induced Fluorescence Spectroscopy (LIFS) to measurement of species concentrations and temperature in flames.

The LIFS method consists of illuminating the gas with a pulsed laser tuned to an absorption line of the species of interest. The species is excited and fluoresces. The fluorescence is observed at 90° to the laser beam, the volume formed by the intersection of the laser beam and the collection optics defining the spacial resolution. If a relationship between the number density of the fluorescing states and the total number density can be found, then the fluorescence is a measure of the total number density. Furthermore, if the fluorescence spectrum is properly interpreted then temperature measurements are possible. Preliminary work with sodium demonstrated the feasibility of saturated LIFS for atomic species. We are now working on diatomic radical species, having recently completed interesting work on OH.

Diatomic molecules present difficulties not found with atomic species. Because of the large number of rotational/vibrational sub-levels available in both the ground and excited electronic states, the nature of rotational relaxation has a strong influence on the fluorescent signal. Although saturating the pumping transition provides some simplification, only in certain limits will the fluorescence signal be unambiguously related to the total number density. Thus one must understand the excitation dynamics if the signal is to be properly interpreted.

We have analyzed the response of OH to laser excitation in considerable detail. By a process of comparing experimental and calculated population distributions we have been able to construct a model for the rotational relaxation rates of the $^2\Sigma^+$ $v' = 0$ state. Using the model, we can in turn interpret other

observed spectra to recover number density and gas temperature.

We feel that laser induced fluorescence spectroscopy has reached a stage of development which warrants its increased use by those interested in observing either atom or diatomic radicals in combustion environments.

MASS SPECTROMETRIC MEASUREMENTS OF THE CONCENTRATIONS OF GASEOUS SPECIES IN REACTIVE FLOW SYSTEMS

(F33615-78-R-2066)

C. Chang and T. O. Tiernan
Brehm Laboratory
Wright State University
Dayton, Ohio 45435

It is well recognized that a thorough understanding of the process of turbulent mixing, ignition and combustion of fuels in flow fields, such as those present in a dump combustor, is vital to the successful design and development of advance air-breathing propulsion systems. The present contractual effort was undertaken for the purpose of developing and implementing a diagnostic method for in-situ measurements of the concentrations of various gaseous species in dump combustor flow fields, utilizing the facilities located at the Air Force Aero Propulsion Laboratory.

The method selected for the present purpose involves the use of a sampling probe-mass spectrometer system. The tasks to be performed under the present project can be cast into four phases as follows:

Phase I. Development and implementation of the present diagnostic

system for in-situ measurements of the concentrations of the simulated fuel (Argon) in the flow field of an APL dump combustor. Through a detailed profiling of the concentration distribution of the simulated fuel within the combustor flow field under various experimental conditions some in-depth information on the fuel-air mixing phenomenum can be gained.

Phase II. Development of methodology for monitoring several gaseous species of interest in the active combustor environment, including N_2, O_2, CO, CO_2, H_2O and fuels. The design and fabrication of a gas calibration system is required in connection with these monitoring studies. The development of procedures for detecting the components of each standard mixture prepared, and the determination of the mass spectrometer signal response for these components over a wide range of mixture concentration are to be conducted. Possible interferences from other compounds which are expected to be present during a typical combustor experiment are also to be assessed.

Phase III. Evaluation of the gas monitoring system. Tests of this system are to be conducted utilizing a flat-flame burner, for which the flame characteristics and the combustion product distributions have already been well established. These experiments are expected to yield test data useful especially in the design of the sampling probe to be used in the future combustion tests.

Phase IV. Interface of the gas monitoring system with the APL dump combustor facilities. Sampling and monitoring of gaseous products from actual combustion tests are to be conducted in this phase.

During this presentation some progress for phases I, II, and III of the present project will be briefly reviewed.

COMPARISON OF RAMAN SCATTERING METHODS FOR COMBUSTION DYNAMICS MEASUREMENTS/CONTRACT F49620-77-C-0094

M. Lapp, Principal Investigator
M. C. Drake, Chemist
C. M. Penney, Physicist
S. Warshaw, Physicist

General Electric Company
Corporate Research and Development
P.O. Box 8, Schenectady, NY 12301

Through steady development and refinement, modern combustion devices have reached high levels of performance. However, increasingly demanding requirements on these devices, such as improved utilization of diverse fuels possessing less stringent specifications, have pushed traditional engineering approaches to combustion design to the limit. New design techniques and aids can arise most readily from the increased understanding and insight obtained through detailed measurements of fundamental properties of laboratory and prototype combustors, and from the combustor models which can then be constructed and tested through use of these basic data.

The work presented here concentrates upon exploration of the limits of measurement capability for a promising diagnostic technique for the determination of flame temperature, viz, vibrational Raman scattering. The major questions addressed involve experimental accuracy, validity of the resultant data (including possibilities for misinterpretation from non-random influences), accessibility of data in the presence of measurement difficulties (such as flame luminosity and sooting), and, ultimately, a comparison of these areas with the results of similar studies for CARS (coherent anti-Stokes Raman spectroscopy, currently under investigation in combustion studies at AFAPL).

The foundation of this research program is based upon use of well-characterized and reproducible burner flows for both laminar premixed and turbulent diffusion flames. The selection, fabrication and testing of burners to produce these flames has now been completed. The laminar premixed flames are produced on a 2.5-cm-diameter horizontal porous plug burner assembly, in which an additional porous plug, coaxial with the burner head and connected to a vacuum line, holds the flame horizontal. The turbulent diffusion flames are produced on a 3-mm-diameter fuel tube contained within a 15 cm X 15 cm square test section (with optical viewing windows approximately

1 m long), through which a coflowing air stream passes. This air flow is induced by a fan at the exhaust. Aerodynamic design of the tunnel has resulted in low levels of background turbulence and good flow uniformity, as measured by hot-film anemometry, pitot tubes, and static pressure taps. The turbulent combustion tunnel is movable in three dimensions (through use of an axial "trombone" section coupled with lateral and vertical bellows motion well downstream of the test section) in order to permit the use of fixed-bed optical diagnostics.

The major accomplishments during this past reporting period include efforts related to (1) the combustor facilities, (2) new Raman data acquisition, and (3) data interpretation. (1) The first of these - the establishment of the new fan-induced co-flowing jet combustor tunnel for studying turbulent diffusion flames - has been described in the preceeding paragraph. This tunnel is now fully operational.

(2) Preliminary Raman temperature data have been obtained for a lightly sooting premixed laminar fuel-rich propane-air flame. These data were obtained using the nitrogen vibrational Stokes/anti-Stokes intensity ratio as the temperature indicator. Raman data were acquired for each channel through use of electronic sample-and-hold circuits to measure the electrical signals present just before and just after appearance of the Raman source laser pulse, in order to reduce spurious signals. Data that were clearly distorted, corresponding to test zones containing particles hit by the laser beam, were discarded using discrimination based upon the absolute signal level. (These discarded radiation signals could have arisen from leakage of Mie-scattered light within the spectrometer or from laser-induced incandescence or fluorescence.

While the use of vibrational Raman-scattering for measurements in flames containing appreciable amounts of soot is clearly difficult, our work to date indicates that extension of the range of applicability of this technique may be possible through the use of conditioned sampling. Here, we are exploring the use of laser velocimetry to detect the appearance of a significantly large soot particle in the Raman test zone. The resultant velocimetry signal, suitably delayed for the time required for the soot particle to leave the flame test zone, would then be used to initiate firing of the pulsed laser for Raman data acquisition.

(3) Background radiation effects will always present a limitation to experimental accuracy in determining temperature from Raman data, but continued improvements in spectroscopic techniques and analysis have ameliorated the problem. In related work, experimental accuracy has been improved through a detailed analysis of the influence of the chosen fixed spectrometer exit slit widths upon the temperatures found from the temperature-sensitive vibrational Raman spectral contours which must pass through these exit slits. (It is not possible experimentally, or desirable in principle, to make these slits wider than the widest Raman profile expected; therefore, some of the Raman-scattered light is not detected at the highest temperatures encountered.)

A measure of the validity of the Raman data is being explored by comparison of simultaneously-obtained nitrogen concentration and temperature data with values predicted by equilibrium calculations for these state variables at various values of flame stoichiometry. This method can be extended to comparison of all measurable concentrations - such as unburned fuel, oxidant, or product gas - with temperature. The present work has been carried out for a hydrogen-air flame.

If these temperature-concentration data pairs cannot be fit at some value of stoichiometry, the departure must be ascribed to experimental inaccuracy or to a failure in computational assumptions, such as isothermal test volume, equilibrium flame chemistry, unity Lewis number, etc. These validity tests show potential for improving confidence in Raman-acquired temperature data.

DEVELOPMENT OF COMBUSTION DIAGNOSTICS AND APPLICATIONS TO TURBULENT COMBUSTION/AFOSR F49620-78-C-0026

R. K. Hanson and C. T. Bowman

High Temperature Gasdynamics Laboratory
Mechanical Engineering Department, Stanford University
Stanford, California 94305

1.0 Introduction

Increasing demands on Air Force combustion systems have stimulated new interest in turbulent combustion processes and in the development of new laser-based diagnostics for turbulent combustion studies. This presentation will describe work underway at Stanford to develop and apply tunable lasers for measurements in combustion flows.

Tunable lasers are well-suited for in situ absorption spectroscopy measurements of species concentrations and temperature in combustion gases whenever line-of-sight measurements are appropriate. These lasers also are a powerful tool for determining spectroscopic parameters needed to describe the spectral characteristics of radiation from high temperature gases, such as found in engines, exhausts and plumes. We are utilizing two different tunable laser systems in our studies -- a tunable infrared diode laser and a tunable ring dye laser. These lasers serve as a source of narrow-linewidth radiation whose wavelength can be rapidly modulated to perform fast, high-resolution absorption spectroscopy. The complete fully-resolved absorption line profile of an individual molecular transition can thus be quickly recorded, and from this one can infer the partial pressure of the absorbing species and the lineshape parameters describing the absorption line. Using tunable infrared lasers temperature can be determined by measuring the relative absorption in adjacent lines originating from different vibrational levels. Tunable laser absorption spectroscopy also should be applicable to two-phase flows in that modulation of the laser wavelength on and off an absorption line should provide discrimination against beam blockage effects. The ability to rapidly modulate the laser suggests that tunable laser techniques also can be applied to studies of transient combustion phenomena.

2.0 Results

During the past year, experiments have been conducted in the steady postflame region of a laminar, premixed, flat-flame burner operating at atmospheric pressure. Measurements of temperature

and CO species concentrations have been made using tunable diode laser absorption spectroscopy to demonstrate the utility of this combustion diagnostic technique. The measurements involve rapidly scanning the narrow-linewidth diode laser across individual vibration-rotation absorption lines in the 4.6 micron fundamental band of CO to record fully-resolved absorption line profiles. This information (obtained in times as short as 50 microseconds) has been used in infer both gas temperature and the concentration of CO. A conventional microprobe sampling system was used to measure CO and CO_2 concentrations for comparison with the laser measurement. Thermocouples were used to measure temperature for comparison with laser-based measurements. Results in methane-air flames show good agreement.

Experiments also have been conducted to evaluate the feasibility of tunable diode laser measurements in fluctuating and particle-laden combustion flows. In the first set of experiments, a rotating valve was used to introduce 60 Hz fluctuations in equivalence ratio in a premixed flame stabilized on a slot burner. A series of absorption records were obtained in these flames which confirm that tunable diode laser absorption techniques can track species concentration and temperature fluctuations in combustion gases. The slot burner also was used in a series of experiments to demonstrate the utility of tunable laser absorption as a measurement technique in sooting combustion flows. Operation of the slot burner with rich premixed C_2H_2-air produces highly luminous sooting flames, with estimated soot particle number densities of 10^9 cm^{-3}. In these experiments, the laser beam propagates through the flame, and the wavelength is tuned across the full width of an absorption line of CO. This wavelength modulation provides a simple means of discriminating against the continuum extinction of the particulates. The result of a single measurement is a fully-resolved profile of one or more CO absorption lines, from which can be inferred the CO concentration and temperature.

An important objective of the research program is the application of tunable laser absorption spectroscopy and other diagnostic techniques to turbulent reacting flows to study the coupling between the fluid dynamic and chemical processes. This phase of the program will be carried out in a recently-constructed two-dimensional reacting shear flow facility. Tests have been conducted on non-reacting flows to characterize the inlet flow conditions and the flow field structure in the mixing layer using conventional pitot probes and hot wire anemometry.

INVESTIGATION OF LASER INDUCED FLUORESCENCE AND LDV FOR MEASUREMENTS OF PARAMETERS IN COMBUSTION ENVIRONMENTS

D.W. Sweeney, W.H. Stevenson,
and H.D. Thompson

School of Mechanical Engineering
Purdue University
W. Lafayette, IN 47907

Two on-going research projects at Purdue University in combustion diagnostics are described. In the first project saturated fluorescence is used to measure OH radical concentrations in atmospheric pressure methane-air flames. A Nd-YAG pumped dye laser is used to excite an isolated rotational transition. The resulting fluorescence signal can be analyzed spectrally and temporally to study the excited state rotational distribution. It is found that steady state is not established throughout the upper rotational levels, although the directly excited upper rotational level remains approximately in steady state during the laser pulse.

The second project considers quantitative evaluation of LDV measurements in turbulent and mixing flows. A variable probe volume laser velocimeter has been designed, built, and is being used to experimentally study bias errors in highly turbulent flows. Preliminary experimental measurements verify a velocity bias for ensemble averaged data. The results of a detailed computer prediction for two-dimensional flow over a rearward facing step (i.e., dump combustor configuration) along with experimental pressure and LDV measurements will be reviewed.

Coherent Structures in Turbulent Flames by Laser Anemometry

Contract/Grant Number AFOSR-77-3414

Norman Chigier and Andrew Yule

University of Sheffield
Department of Chemical Engineering and Fuel Technology

Sheffield, England

Advanced diagnostic techniques for turbulent flames are being developed at Sheffield University to assist the U.S. Air Force in the development of advanced air-breathing engines and other Air Force combustion systems. Reliable measurements of significant parameters in turbulent reacting flows are obtained in hostile combustion environments using laser diagnostic techniques and miniature probes. Measurements provide an accurate data base for formulation and evaluation of mathematical models. The specific objective of the study is to develop more sensitive, selective, precise, reliable and high frequency response diagnostic methods for measuring important parameters in jet engine reacting flow environments. The feasibility of using laser Doppler anemometry for obtaining high spatial and time resolution as well as measurements of particle size and velocity simultaneously has been demonstrated in practical combustion environments. The combination of experimental and analytical studies will help to reduce the development time and cost of air-breathing propulsion systems.

The aim of the research is to increase fundamental understanding of turbulent combustion in gas diffusion and spray flows related to propulsion systems; with particular emphasis on the roles of large eddies (coherent structures) in the turbulence. This objective requires the development of high resolution measurement techniques. Progress in the development and application of techniques has been made for the measurement of particle size and velocity by laser anemometer, temperature by computer interfaced thermocouples and flame ionization by ionization probes. Initial results of the investigation have been derived for the two major areas: axisymmetric diffusion flows and fuel sprays. The importance of the initial, near field, region of the diffusion flame and the influence of heat release in the transitional flow are investigated. The initial research with fuel sprays, using laser anemometry, shows the importance of being able to measure gas velocity, particle velocity and particle size, simultaneously. This permits derivation of temporally averaged size distributions and turbulence-droplet interaction. The initial experiments have clearly demonstrated the importance of large scale structure, its development from transitional structures and the interaction between combustion and the formation of these structures. The new LDA system has clearly demonstrated the interaction between the turbulent gas flow and the droplets in the fuel spray.

The first 20 diameters of flow in a jet flame have been mapped in detail from radial traverse measurements, providing mean, rms and pdfs of velocity, temperature and flame ionization levels. Velocity measurements have also been made in the corresponding non-burning flow to obtain information on flow structure in the initial region of the jet. The real-time LDA system for the diffusion flame study has been improved by installing a new beam-splitter and Bragg cell and a more sensitive photomultiplier. The initial measurements have been correlated with colour-schlieren high-speed films. These clearly show vortex formation, coalescence, growth of three-dimensionality and interface burning regions. A comparison of the cold and burning flows shows very significant differences attributable to dilatation and increased viscosity. Progress has been made in the development of data analysis techniques for conditional sampling of flame structure.

An Interim Scientific Report "Coherent Structures in Turbulent Flames", was submitted to AFOSR in October 1979. A paper based on this report will be presented at the AIAA 18th Aerospace Sciences Meeting, Pasadena, January 1980. Experimental data are presented for a turbulent jet flame of $Re = 10^4$ using propane gas. High-speed cine photography shows the detailed structure in the first 20 diameters of the flame. Laser anemometer measurements in burning and non-burning conditions are presented showing very significant changes in mean velocity and turbulence intensity. The effect of change of seeding concentration on LDA measurement is demonstrated. Ion current profiles show how thermal expansion causes change in mean velocity profile. Peak frequencies measured by laser schlieren and high-speed cine are shown to be in agreement. Initial results of a computer model for a cylindrical mixing layer instability are shown for two time delays after initial disturbance.

MEASUREMENT OF TURBULENCE IN COMBUSTION SYSTEMS BY RAYLEIGH SCATTERING

F44620-76-0083

Lawrence Talbot

Department of Mechanical Engineering
University of California
Berkeley, California 94720

1. INTRODUCTION

The need for an improved understanding of the effect of turbulence on chemically reacting flows has long been recognized. However, the inherent experimental and theoretical difficulties associated with these flows have continued to impede progress towards the development of models which could eventually be used in design situations to aid our understanding of practical combustion. New measurement techniques, notably laser Doppler velocimetry (LDV) have improved the situation, but the experimental data available is still sparse compared with data for other turbulent flows. The theoretical picture for turbulent flows with combustion is complicated by the necessity of introducing density variations in the theoretical specification of the problem. Numerical models for turbulent flows in which the fluid may be considered incompressible now successfully predict details of fairly complex flows (Ref. 1). However, these models are not easily applied to combustion problems since the introduction of variable density results in terms which have no counterpart in the incompressible models (Ref. 2).

Rayleigh scattering has been shown to be a reliable and accurate method of determining gas density under typical combustion conditions (Refs. 3,4,5).

2. FLAME PROPAGATION IN GRID INDUCED TURBULENCE

Experimental Facilities

The basic optical systems for single point Rayleigh scattering and laser-Doppler velocimetry (LDV) are used in both experiments and are described in detail in Ref. 7. To facilitate the use of these optical systems, a computerized data acquisition system based upon a Digital Equipment Corporation (DEC) PDP 11/10 has been developed to record Rayleigh scattering signals from an electrometer and the processed LDV signals from a Thermo-Systems 1090 frequency tracker.

In all studies, the experimental apparatus is mounted on an 3-axis traverse mechanism so that the optical system may remain stationary. The 3-axis traverse is operated by separate stepper motors which are computer-controlled and scan flow field position for Rayleigh scattering and LDV measurements automatically. Measurements are obtained using an 8-channel, 12 bit A/D converter. Samples may be acquired at a constant sampling rate through clock control or individual samples may be initiated by a separate interrupt input by the user. In the latter mode the time between samples is continuously monitored by the clock. Raw data may be stored in disk memory files or on 7-track magnetic tape for post-processing either with the PDP 11/10 or the Lawrence Berkeley Laboratory CDC 7600.

Measurements

The importance of the effect of turbulence on flame propagation is attested to by the numerous studies in which flame speed is correlated with the scale and intensity of turbulence. Recent reviews of such studies may be found in Refs. 8,9. Our study uses Rayleigh scattering and LDV as diagnostics on a V-shaped C_2H_4-Air flame stabilized on a rod. Initial LDV measurements downstream of a bi-plane grid of mesh size 5 mm have now been completed for free stream velocities ranging from 2-7 m/s and equivalence ratios ranging from 0.55 to 0.75. In Figure 1, LDV measurements of the mean and rms levels of the streamwise velocity component are presented at a distance 16 mesh lengths downstream of the grid. The grid Reynolds number of 700 is slightly above the lower limit reported in Ref. 12 for grid turbulence. The particle arrival rate was approximately 8000 per second and the sampling rate was 2000 samples per second. The mean and rms levels of the velocity at $y = 16$ corresponds to the levels inherent in the flow through the grid without a flame. The position of the flame holder corresponds to $y = 0$. As the flame front is approached and the gas density drops, the flow is accelerated. A sharp rise in the fluctuation level occurs at the flame front. Beyond the reaction zone, the fluctuation level drops sharply with the turbulence intensity decreasing below the level induced by the grid. Theoretical predictions of Ref. 11 indicate net turbulent kinetic energy may either be produced or destroyed by the flame front depending upon competing production terms related to mean shear and loss terms related to mean flow dilation. Our data now indicate that a consideration of the effect of the wake of the flame holder on the flame front is crucial to the interpretation of such phenomena. Rayleigh scattering and LDV measurements are to be continued for varying grid Reynolds number and equivalence ratios to determine combustion parameters which influence these interactions.

3. INTERACTION OF A VORTEX STREET WITH A PLANE FLAME FRONT

In order to more precisely measure the effect of flame front curvature and turbulent eddies on flame propagation a study was undertaken of the interaction of a plane flame front with the vortex street shed from the wake of a cylinder (Ref. 6). This study has the advantage that phase-locked averaging techniques may be used to map the changes in the entire flow field as a function of time since the shed vortices have definite frequency and phase relations (see e.g., Ref. 10). Preliminary measurements have shown that Rayleigh scattering can be successfully used to measure density fluctuations due to the interaction of the vortex street with the flame front.

The ability to use phase-locked averaging techniques in this experiment depends on the availability of a reference probe which can be used to give a time signal which is locked in phase with a given position of the vortices.

In Figure 2, profiles across the flame front of the mean and rms fluctuation level of the streamwise component of velocity are reproduced for a position 30 mm downstream of the vortex generating rod. The flame holder is positioned at $y = 0$. The local peak in the rms, seen at $y = 14$ mm, is due to the passing vortex just outside of the nominal position of the flame front. The local minimum in rms at $y = 18$ mm corresponds to the minimum rms disturbance due to the wake of the generating rod. Without these vortices, the rms level is approximately 1%. Preliminary results indicate that both the mean velocity profile as well as the shape of the vortices are distorted by the flame-vortex interaction. Phase-locked measurements of these phenomena as well as density measurements are now being completed.

4. FUTURE RESEARCH

The development and application of Rayleigh scattering and laser Doppler velocimetry to turbulent flows with combustion is to be continued. We plan to extend our present capabilities of Rayleigh scattering and laser Doppler velocimetry to include:

1. Two-point correlations of density;
2. Single-point cross-correlations of velocity;
3. Single-point cross-correlations of density and velocity;
4. Two-point correlations of velocity.

These new techniques will be applied to the studies of flame propagation in grid-generated turbulence and the interaction of a vortex street to a plane flame front.

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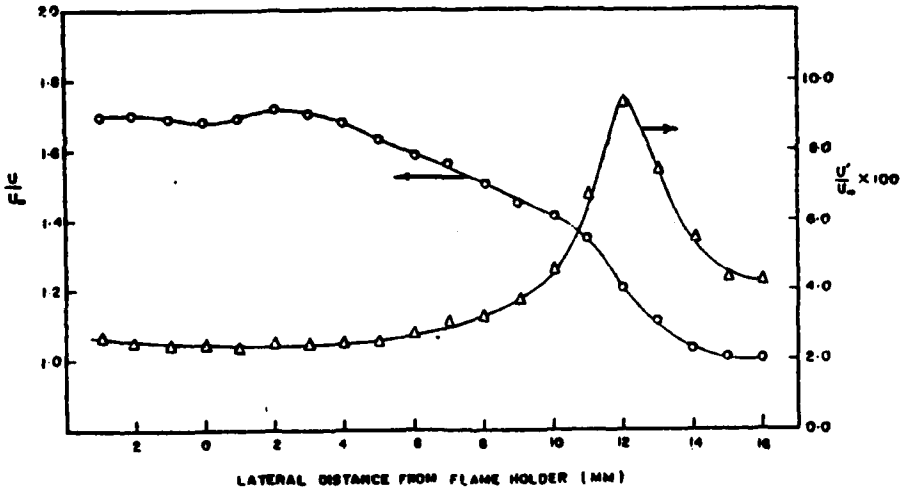

Figure 1. Mean and rms velocity, u, in grid generated turbulence

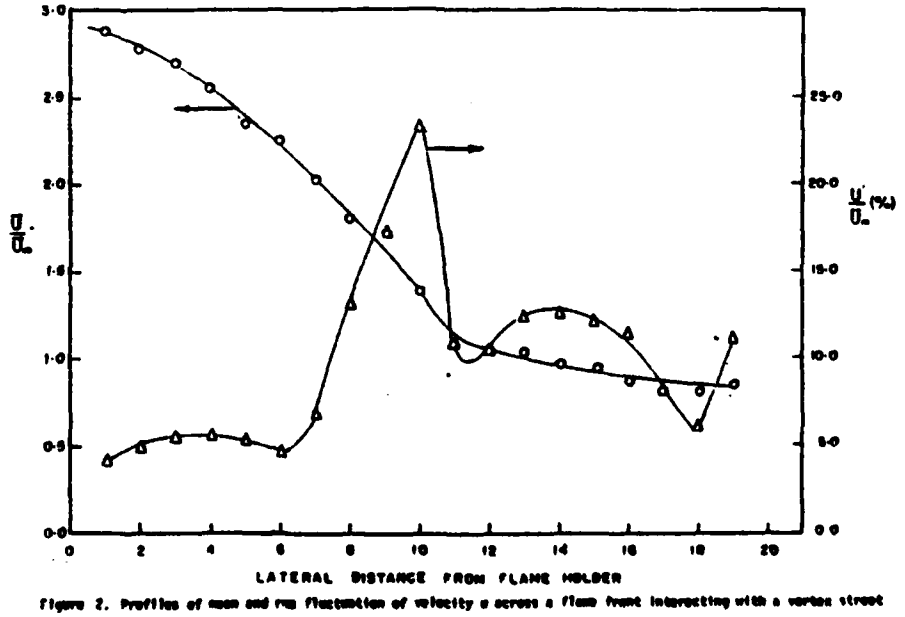

Figure 2. Profiles of mean and rms fluctuation of velocity a across a flame front interacting with a vortex street

IMPROVED FLOW VISUALIZATION BY USE OF RESONANT REFRACTIVITY
(AFOSR-79-0058)

Daniel Bershader

Department of Aeronautics and Astronautics
Stanford University

Stanford, California 94305

The importance for Air Force R&D purposes of improving the sensitivity of fluid and combustion flow visualization methods is self-evident. Refractive methods, especially interferometry, shadow and schlieren techniques, have been especially productive because of their quantitative capability and rather high intrinsic sensitivities. However, these are limited by the values of the specific refractivity of air and other diatomic gases, especially in the visible spectrum. Thus, as of now, we cannot obtain sufficient detail in attempts to visualize portions of rocket plume and exhaust flows, weak vortices in aircraft wakes, turbulence details in boundary layers and audio-frequency sound waves for purposes of noise studies.

Approach in the present work has been to determine the feasibility of utilizing the highly enhanced specific refractivity of sodium vapor near its ground-state resonant wavelength to achieve a one- or two-order of magnitude increase in flow visualization sensitivity. Injection of a small amount of such vapor (between $1{:}10^3$ and $1{:}10^4$) in a carrier gas such as nitrogen or argon would achieve the desired result with a dye-laser light source suitably tuned to a near-resonant point. The latter has to be judiciously chosen in order to optimize the trade-off between resonant refraction and absorption.

The work to date has included (1) a successful experimental calibration program to verify quantitatively the enhanced refractivity in the near-resonant region; (2) a theoretical determination of the shape of both the refractive and absorptive profiles in the near-resonant region, taking into account the effects of both collisional and Doppler broadening (Voigt profile analysis); and (3) a set of absorption studies to examine more closely the simple pressure-dependence assumptions in collisional line broadening, as well as possible interference effects from the molecular spectrum of Na_2 in the near region.

Results of decisive importance for the successful application of this method in flow systems include: (1) The tradeoff between absorption and refraction effects in the near-resonant region is a favorable one because the absorption coefficient falls off faster than the specific refractivity in that region (around 5Å to 10Å off resonance). Thus, at 5880Å (10Å off resonance), the ratios of specific refractivity of sodium vapor to the non-resonant value

for air is 4500, this result at a wavelength where the laser beam retained considerable intensity after absorption through a one-meter path of (pure) sodium vapor at a pressure around 10 torr; (2) the fact that further refractive enhancement around a factor of 15 would occur when sodium is injected into the diluent or carrier gas, because the heterogeneous collisional broadening due to sodium-diluent collisions is less severe than self-broadening in pure sodium vapor (sodium-sodium collisions); (3) a second trade-off in the near-resonant region where the spectral effects of the few per cent of Na_2 may be ignored because of the magnitude of the atomic sodium resonant behavior; (4) indications that a stronger dye-laser light source (present pulsed laser develops a peak output power of 31KW, and an output energy of 155 μ-Joules) would permit operation several Å closer to resonance, with associated further enhancement of refractive behavior. E.g., the specific refractivity improves by another factor of 3 between 5880Å and 5887Å.

The calibration results have been reported,[1] and together with the major analytical results[2] indicate the feasibility of the method. The technique of injection of small amounts of sodium vapor from an oven at about 500°C into a flow device has already been used by research chemists and others, but needs further development in aerodynamic applications. In other words, this program is ready for a pilot-model "hardware phase." For application at higher temperatures the procedures may be simpler yet: At present, our laboratory is experimenting with injection of large amounts of sodium iodide into a laboratory flame in the attempt to assess whether a minimum atomic density can be achieved for use with resonant optics; that work is still in progress.

TABLE

NEAR-RESONANT VALUES AND RATIOS OF REFRACTIVITY

[Å]	5870	5875	5880
$K_{r_{Na}}$ [m^3/kg]	0.546	0.698	1.0360
$K_{r_{Na}}/K_{o_{Na}}$	134.8	172.4	256
$K_{r_{Na}}/K_{o_{Air}}$	2374	3034	4504

NOTE: The Gladstone-Dale constant is the specific refractivity defined by $K = \frac{n-1}{\rho}$, where n is the refractive index and ρ is the mass density. Subscript o represents non-resonant value.

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APPLICATION OF 3-D IMAGE RECONSTRUCTION TECHNIQUES FOR ANALYZING COMBUSTION DYNAMICS

R. V. Denton
Systems Control, Inc.
Palo Alto, Calif. 94304

Image reconstruction (also known as computerized tomography) has been applied extensively in medicine and to a lesser extent in nondestructive evaluation. It is suggested that these methods can also be applied to analyze combustion dynamics, starting, for example, from multiple angle laser measurements of the combustion process. In particular, it is shown that the measurements can be used in a new three-dimensional image reconstruction algorithm to obtain three-dimensional images of the combustion volume at various snapshots in time during the combustion process. Some of the resolution issues are also discussed.